

# Annual Report

2015-2016



**Centre for Doctoral Training in  
Theory and Simulation of Materials**

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We would like to acknowledge the contributions from the editors of previous years, who left us an excellent template which set the foundations for this year's report.

London, November 2016

The back cover is a modified version of the original design by Farnaz Ostovari

*“No one can whistle a symphony. It takes a whole orchestra to play it.”*

—HALFORD E. LUCCOCK, as recited in 'Roadblocks to Faith' by J.A. Pike and J. M. Krumm, 1954

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# Director's Foreword

It is a great pleasure to write the foreword for this, the fifth edition of the TSM-CDT annual report. The CDT was founded in 2009 with a mission to create a new generation of scientists and engineers with the theoretical and computational abilities to model properties and processes with materials across a range of length and/or time scales. This year we have welcomed our eighth cohort of students, taking the total number of students in the extended CDT family to over 90, around 30 of whom have graduated and are now counted among our alumni. Reflecting back on the past seven years since we recruited the first cohort of students, there is a great deal to be proud of across a number of different areas.

In science, our mission to bridge length and time scales, and the requirement for projects to have two supervisors with complementary expertise, has led to ambitious, multi-disciplinary research that straddles traditional disciplinary "silos" and that would not have occurred otherwise. CDT projects have involved over 70 distinct supervisors, not only from the nine participating departments across the Faculties of Engineering and Natural Sciences at Imperial, but also from eight other academic institutions (including King's, UCL, Manchester, Oxford and Cambridge), and ten industry partners (including Baker Hughes, Rolls Royce, the Culham Centre for Fusion Energy and Materials Design Inc.).

In education, we take pride in the way the MSc in TSM has evolved over the years to provide students from different disciplinary backgrounds, including physics, materials, chemistry, engineering and mathematics, the best possible preparation for research in TSM. In the words of our external examiner, Prof Graeme Ackland of the

University of Edinburgh, the MSc is "an excellent programme taking students with Materials Science, Physics or Chemistry backgrounds and teaching them the basics of materials science... The advanced material is challenging for all, up to date and relevant for their future PhD."

In personal development, our aim is to enable students to make the very most of their broad range of skills. The CDT's suite of bespoke transferable skills courses includes personal effectiveness and team working (with Piero Vitelli at Island41), careers (with Adrian Sutton), science communication (with Gareth Mitchell and the BBC), and ethics (with Marianne Talbot from the University of Oxford).

But perhaps what I am most proud of is the students themselves and their achievements. For example, among our 30 or so alumni, around one-third have gone on to further academic research at leading academic institutions, including Imperial, MIT and Cambridge; several others work for multinational companies such as IBM, Rolls-Royce and BAE Systems; many use their skills in data analysis and programming as software engineers in small-to-medium enterprises; and a handful are successful entrepreneurs and founders of tech start-ups.

It is certainly true that our students are our greatest ambassadors and in this annual report (which is an entirely student-led publication), you will see a brief glimpse of the breadth of their activities and the depth of their energy and enthusiasm. Enjoy!

**Arash Mostofi**  
*Director, Centre for Doctoral Training in  
Theory and Simulation of Materials*

# Cohort VII : The MSc experience

**FANGYUAN GU, ANDREW WARWICK** and **LARA ROMÁN CASTELLANOS** recall some of the highlights of their MSc year.

This was both a rewarding and intense year for our cohort. Yes, the MSc course familiarises you with the wide field of materials science, but for us it did much more than that. It broadened our horizons, gave clarity to our academic interests and helped us develop a good group of friends in research. One of the greatest strengths of this CDT is its ability to bring together people from very different backgrounds in an interdisciplinary environment and highlight just how much we have in common. Who would've thought engineers and physicists could get along so well?

The course covered a broad range of interconnected subjects using the language of quantum mechanics to tackle atomic length scales up to continuum mechanics for macroscopic materials. Learning all of this was undoubtedly a challenge, but such situations emphasise the importance of being organised and working together; developing useful skills for any path we may choose to follow during and after the CDT. Anyway, as they say, no pain no gain!



Taking courses was, of course, only part of our MSc year. As a pleasant surprise we found ourselves organising the Christmas party for the whole CDT as early on as the end of the first term. Clearly the older cohorts have put together several events between them and for us to get a taste of this was very rewarding, memorable and fun. We learned much in the way of buying and slicing too much bread, throwing away a mountain of cheese that clearly hadn't gone off and also mis-managing our entire food order that Miranda and Veena had to rescue in one night.



As one of the first events in the year to bring the whole cohort together, it marked the beginning of getting to know each other outside of science. It did end up being a great success and made for both a really enjoyable celebration and a nice break away from our work.

The CDT also arranged for us to visit one of our industrial partners, Element 6, at their Global Innovation Centre in Harwell. There we gained invaluable insight into how our technical skills could be applied in a commercial setting. The whole business park felt futuristic and the site of Element 6 itself had a similar atmosphere. In a pristinely modern setting we learned about their diamond synthesis processes and what it is like to work in industry. Later we engaged in a lively discussion surrounding a practical problem they have been recently focusing on.

As per tradition, the MSc culminated in a trip to the EMRS (European Materials Research Society) conference, which this year was taking place in Warsaw. Food and drink were both affordable and came in big portions, which for Londoners was a welcome change, so we knew we were in for a good trip.

At the conference itself there was something for everyone, be it by attending talks or viewing posters across a wide range of subjects. In particular though, our very own Ignacio Bordeau Weldt and Mariana Hildebrand won best poster awards in their respective fields!

One of the best things about the trip was what it did for us as a cohort. After strolling around the city at night, dining in a weirdly fancy communist-themed restaurant (once host to Bruce Willis) and grabbing the occasional drink together, it's safe to say we now have a close-knit group of friends for the remainder of the CDT and beyond.

Everything from the intense studying to the most relaxing moments certainly made for an incredible year. There are even better times to come for Cohort VII, no doubt about it!



# Life and Soul of the CDT

**What were you most excited about before joining the CDT? Was there anything that worried you?**

It sounded like the perfect type of PhD for me, where your supervisor doesn't try to squeeze the most out of you without caring about your personal development and goals. I was not worried by anything, I was excited.

**Nicola Molinari (Cohort V)**

Coming from a physics background, I was most excited to find out how materials problems differed from purely theoretical physics problems. I was worried that they would have nothing in common whatsoever. This worry vanished when I saw how varied the field of materials science is!

**Adam Ready (Cohort IV)**

I was most excited about finally learning "proper" quantum mechanics. Worried about not being good enough to understand it.

**Lars Blumenthal (Cohort VI)**

Ditto.

**Alise Virbule (Cohort VI)**

**Now you're here, what do/did you enjoy the most about the CDT? What have you found most challenging?**

The one thing I've enjoyed the most is the friends I've made. People from all walks of life, from all over the world and from so many different departments and across London! Challenging: the personal issues that sometimes pop up in life are extremely hard to deal with whilst doing something as intense as a PhD.

**Andrew McMahon (Cohort V)**

**Describe your cohort in one sentence.**

A very creative and intelligent bunch of people who are not afraid of taking the initiative and trying something new.

**Lars Blumenthal (Cohort VI)**

If you put us all in one room for a few hours, with pretty much any problem - I think we could create a reasonable solution given the time, so I think we make a decent team!

**Hikmat Hassan (Cohort VI)**

The happy friends of Farnaz. There were quite a few subgroups in our cohort at the beginning, but I think the person that managed to bring us more together as a cohort is Farnaz.

**Nicola Molinari (Cohort V)**

Great personalities with grand opinions about politics, philosophy and life.

**Mitesh Patel (Cohort V)**



**Cohort VI celebrating at their MSc graduation**



## How do you think being in a CDT compares to a normal PhD program?

The CDT provides an outstandingly multicultural group of people that during the first few weeks of the program become your friends rather than colleagues. While nothing blocks you from achieving this with a normal PhD, in my experience the tight bonds that we created by struggling together on problem sheets, organising events, attending courses and through all the other activities in the CDT are quite unique and make you feel part of a family rather than a research group.

**Nicola Molinari (Cohort V)**

The CDT helped me develop lots of skills, not just in research. Doing a lot of outreach activities, such as co-organising a summer school, leading a fundraising campaign, and working with school children, were a challenge but helped me grow as a person. I am also still in the process of establishing the full set of skills required for a computational scientist. Techniques such as obtaining and utilising external libraries, navigating the literature, and distinguishing numerical noise and personal bias from genuine results. A lot of these skills you would also learn in a regular PhD, but I feel that the structure of the CDT definitely nurtured my scientific expertise.

**Vadim Nemytov (Cohort V)**

The strong focus on outreach activities gave me a new perspective on the role of scientists in our society.

**Iacopo Rovelli (Cohort VI)**

The MSc is very valuable as it gives you a solid background in the very broad field of materials science and it allowed me to move into a field I hadn't even heard of before joining the CDT.

**Jonas Vershueren (Cohort VI)**

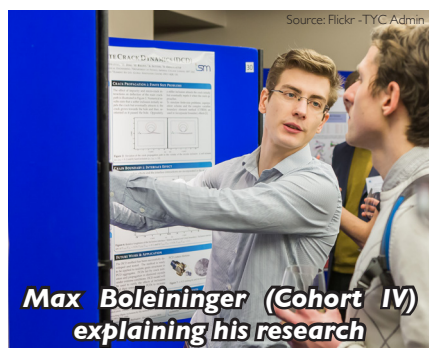
## What would you say to someone applying to the CDT?

The CDT understands that your PhD culminates with an outstanding research dissertation, but the real product is yourself. If you want to make an investment in yourself, this is the place for you.

**Mitesh Patel (Cohort V)**

You will enter a new world of research where you not only get to develop your academic and scientific capabilities but you can work on your social and communicational skills as well.

**Farnaz Ostovari (Cohort V)**



## Tell a story from your time at the CDT.

The evening before a group project deadline, I had invited my team to my place so that we could finish the project. Early on I went for a lie down and fell fast asleep. When I woke up, it was morning, the others had gone and the work was done.

**Hikmat Hassan (Cohort VI)**

I have moved into my identical twin's old department at Imperial, which means I keep having to explain to very confused people that I'm not him - in one case after a very jovial bear hug.

**Jonas Vershueren (Cohort VI)**

# Single-Electron Induced Surface Plasmons on a Topological Nanoparticle

## Research Highlight

**GLEB SIROKI (COHORT VI)**

A little over ten years ago a new class of material was predicted and later realised experimentally. These new materials are insulating inside but have a metallic surface.

Furthermore, their metallic surface is immune to environmental influences, in contrast to the surface of an ordinary metal which becomes covered with an oxide layer when exposed to air. The reason for these exotic properties lies in strong spin-orbit coupling which reorders the electronic levels in these materials.

To understand how they are different from ordinary insulators it is useful to bring an analogy from topology. Imagine a strip of paper - you can connect it to make either a cylinder or a Mobius strip (figure 1). The cylinder would be analogous to ordinary insulators which we are all familiar with. However, in some materials made of heavy elements, spin-orbit coupling can twist the band structure making it distinct from that of ordinary insulators - somewhat like the Mobius strip. These twisted band structures give rise to exotic properties and the materials became known as topological insulators.



Figure 1: The band structure in topological insulators is analogous to a Mobius strip.

So far, scientific interest has mostly focused on macroscopic samples of topological insulators. In particular, large research effort is aimed at employing the metallic surface states of electrons for applications in spintronics and quantum computation. Nanostructures of topological insulators have received much less attention.

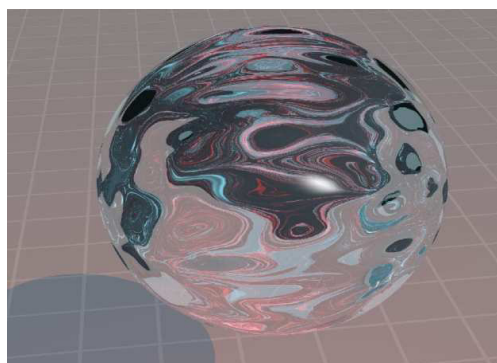


Figure 2: Topological insulator particles can be dark or transparent depending on the wavelength of light [1].

The idea behind the present project was that metallic surfaces should play a more prominent role in topological nanoparticles as they have a larger surface-to-volume ratio. With the help of my supervisors, Dr Vincenzo Giannini, Dr Derek Lee and Prof Peter Haynes, I have discovered this to be the case. Our theoretical calculations (figure 2) predict that even a single electron in a metallic surface state of a topological insulator nanoparticle can drastically change its optical properties. This is surprising given that the nanoparticle consists of hundreds of thousands of atoms. Such an electron can enhance absorption at some wavelengths whereas at others it can completely screen the body of the nanoparticle from the incoming light. These findings may prove useful for areas of THz photonics and quantum information.

[1] G. Siroki, D.K.K. Lee, P. D. Haynes & V. Giannini, *Nat. Commun.*, 2016, 7, 12375.

# Tuning Negative Thermal Expansion by Chemical Control

## Research Highlight

**CHRIS ABLITT (COHORT VI)**

The vast majority of materials expand on heating. Therefore the rare exceptions which contract with increasing temperature – a novel property known as negative thermal expansion (NTE) – are interesting, both from a scientific and a technological perspective.

It is a common problem in engineering that if two materials are coupled together, they may expand differently when they undergo large temperature changes. By understanding and, better still, being able to control the rate of expansion of a material with respect to temperature, we can design new materials with tunable thermal expansion properties.

Controllable uni-axial NTE (NTE along one dimension) has recently been demonstrated over a large temperature range in a layered perovskite material, known as a Ruddlesden-Popper oxide, with chemical formula  $\text{Ca}_{3-x}\text{Sr}_x\text{Mn}_2\text{O}_7$ . By varying the proportions of calcium and strontium in the

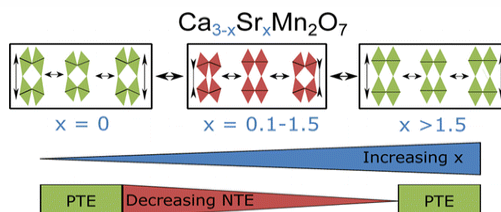


Figure 2: By replacing calcium in the structure with strontium we were able to tune the magnitude of NTE [1].

structure, we were able to exploit the competition between different crystal phases to tune the thermal expansion from pronounced NTE right through to positive thermal expansion.

This work was a large collaboration, comprised of our group at Imperial College London alongside allies at Oxford University, Diamond Light Source and institutions in Korea and the US. Between us we have synthesised the material and demonstrated the effect, measured its crystal structure, and performed computational simulations.

My contribution to the work was to use density functional theory (DFT) calculations to show that a particular type of atomic vibration, which consists of the tilting of rigid octahedral units in the structure, could be driving the NTE. I also showed that, when varying the amount of strontium in the compound, the change in frequency of these vibrations correlates with the change in the rate of the experimentally measured thermal expansion.

These results pave the way to being able to understand NTE in perovskite materials and to design materials with controllable thermal expansion.

[1] M. S. Senn, C. A. Murray, X. Luo, L. Wang, F. Huang, S. Cheong, A. Bombardi, C. Ablitt, A. A. Mostofi, and N. C. Bristowe, *J. Am. Chem. Soc.*, 2016, 138 (17), 5479.

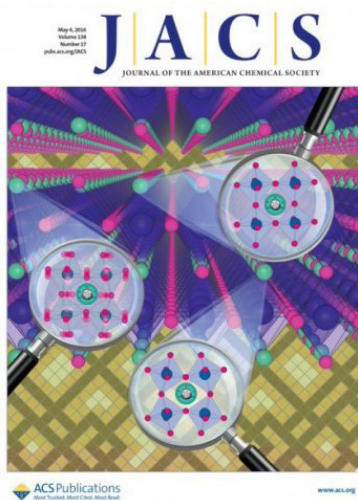


Figure 1: This work has been published in *Journal of the American Chemical Society* [1].

# Optimising Water Transport through Graphene-Based Membranes

## Research Highlight

In modern engineering practices nanotechnology is becoming increasingly popular. A lot of resources are being dedicated to understanding nano phenomena and how to best apply them to real world problems. One of the main areas studied is nanofluidics. A significant discovery was the extremely fast water flow through carbon nanotubes (CNTs), as they can ensure high rejection rates whilst simultaneously providing fast water permeation. This kickstarted a large array of research projects investigating its possible application to cheap and efficient water purification.

As CNTs are difficult and expensive to produce, research has deviated towards the investigation of graphene sheets in reverse osmosis membranes. Experimental research suggested that graphene oxide, an easily producible and inexpensive material, showed very high water flow whilst being impermeable to helium gas.

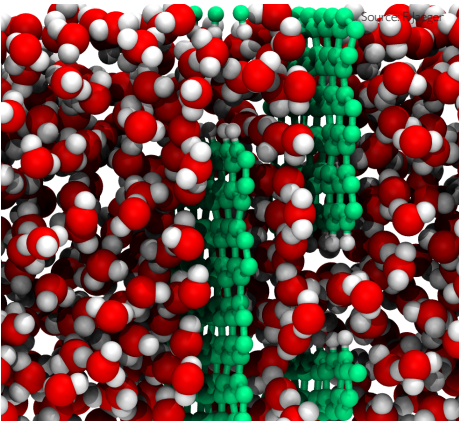


Figure 1: Water molecules passing through a graphene-based membrane.

In our research we aimed to investigate what may cause such high flow rates and how the rejection behavior of the membrane can be maximised whilst retaining the high throughput [1]. We looked at simplified graphene oxide-like mem-

**FREDA JAEGER (COHORT V)**

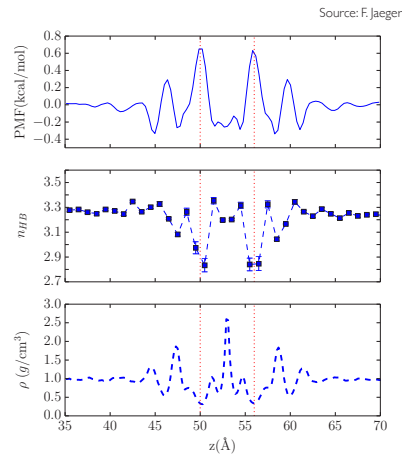


Figure 2: Energy cost associated with traversing the membrane and breaking hydrogen bonds.

branes, consisting of layered graphene sheets with slits, and considered a variety of factors that together paint a picture of the water transport. Our analysis showed that an energy barrier exists for water molecules passing through a slit, which is significantly higher for smaller slits. This occurs due to the breaking and reforming of hydrogen bonds, which is necessary to allow water molecules to enter the membrane and form a structurally different system within it. We further showed that water molecules actually spend a significant time within the membrane, confirming that no preferential fast transport in the confined environment exists, contrary to that previously suggested.

The main conclusion from our work is that the size of the slits in the membrane should not be used to filter unwanted components in the liquid due to the high energy barrier associated with this process. Instead the distance between the sheets themselves, which can be modified through linkers, should play that role.

[1] J. Muscatello, F. Jaeger, O. K. Matar, and E. Muller, *ACS Appl. Mater. Interfaces*, 2016, 8 (19), 12330.

# Strong Room Temperature Coupling in Nano-Plasmonic Cavities

## Research Highlight

Strong coupling is the coherent exchange of energy between light and matter. The conditions needed for strong coupling to take place are difficult to achieve, usually involving some kind of cavity. Not only do you require a small spatial confinement of the light field, you also need to satisfy the coherence condition between the light and matter for the strong coupling to take place. One system that has shown excellent promise in achieving these conditions is the gold nanoparticle-on-mirror (NPoM) geometry (figure 1), which exploits the properties of plasmonic materials. A plasmon is a mixed light-matter surface state. Upon exposure to a polarized electric field in the y direction, a hot spot is created in the gap between the NP and gold mirror. Then, upon placing a molecule/spacer in the gap, strong coupling may be achieved between the molecule (quantum emitter, QE) and the light field.

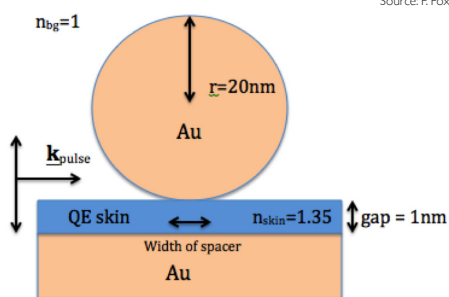


Figure 1: The geometry of the gold NPoM investigated.

Traditionally one would try to model the above system using classical light fields and classical narrow bandwidth harmonic oscillators to model the molecule. What we were able to do was model the whole system semi-quantum mechanically [1]. The field was modeled classically, whilst the quantum emitters were modeled quantum mechanically, using the Maxwell-Bloch equations. We were able to show that single emitter strong coupling

**PETER FOX (COHORT V)**

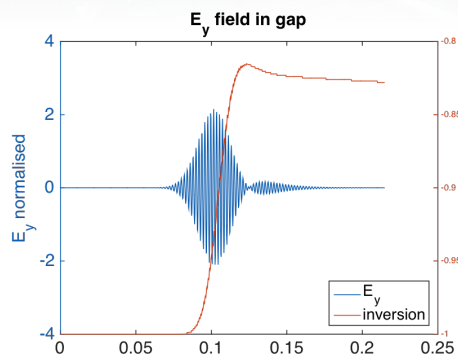


Figure 2: Damped Rabi oscillations in the  $E$  field in the centre of the gap. The oscillation starts at  $\sim 0.125$  ps. [1]

was achievable with realistic parameters for the quantum emitters.

This research was the result of a successful collaboration between our plasmonics group here at Imperial College London and experimentalists at the University of Cambridge. They were able to achieve remarkable results using a guest-host chemistry setup explained in more detail in the paper. We were able to back up their results in a semi-quantum mechanical context; particularly the fact that single molecule strong coupling was achievable at room temperature. Also, we were able to explicitly show the Rabi oscillations between the light and the QEs by plotting the electric field in the centre of the gap (figure 2). The Rabi frequency of oscillation is the frequency at which energy is alternating between light and matter. My primary tool for modelling the system was the group FDTD (finite difference, time domain) code.

As part of the collaboration I was invited to go on a Winter School trip at a top ski resort, organised by Cambridge in the beautiful French Alps.

[1] R. Chikkaraddy, B. de Nijs, F. Benz, and S.J Barrow, O.A Scherman, E. Rosta, A. Demetriadou, P. Fox, O. Hess and J.J Baumberg, *Nat. Commu.*, 2016, 535, 127.

# TSM Annual Conference

**MAHDIEH TAJABADI EBRAHIMI** (Cohort IV), **PREMYUDA ONTAWONG** (Cohort V) and **LUCA CIMBARO** (Cohort VI) report.

This June, members of the CDT gathered for the third annual TSM conference. This event constitutes one of the few meetings of the entire CDT and thus is a time to celebrate the hard work carried out by students from across the centre throughout the year. To join the students, staff and team of directors, this year's meeting also played host to members of the International Advisory board, including guest speaker from Materials Design Inc. Dr Erich Wimmer.



As per tradition, Cohorts V and VI presented academic posters summarising their research, whilst the most senior cohort, this year Cohort IV, narrated the trials and tribulations of their PhD in a series of 15 minute talks. This left the latest reboot, Cohort VII, as judges for the hotly-contested prizes for best poster and oral presentation. After a day filled with riveting talks, broken up by a buffet lunch and poster session, which set the scene for many an insightful discussion, Freda Jaeger (Cohort V) was awarded the poster prize for her display on water transport through graphene (see Freda's research highlight) and Max Boleininger (Cohort IV) snatched the presentation prize for his interactive talk comparing fast electrons to water spilling out of a glass.

Further prizes were then awarded, including the Sutton prize for academic achievement in the

MSc (won by Gleb Siroki, Cohort VI) and the prize for an outstanding contribution to the life of the CDT (Farnaz Ostovari, Cohort V), amongst others. It was heartening to hear accounts of the many extra-curricular and academic achievements from members in all sections of the CDT.



After these awards had been handed out, Dr Wimmer, the keynote speaker, gave a presentation on his illustrious career path. Starting out as a young researcher, with intellectual run-ins with graphene and hybrid functionals (before they were cool) Erich spent a period working at Cray supercomputers and now finds himself as chairman of Materials Design. We found the talk to be an inspirational account of how a theoretical scientist can incorporate computational tools to benefit both society and scientific research while establishing an entrepreneurial business.

As always, the third TSM conference was a student-led event, with organisers from all four cohorts. Premyuda (Cohort V) perfectly captures the CDT spirit when she describes the conference as "a very family-like event". She continues "The presentations of the students were impressive and it was great to see how a group of people who have done the same MSc have ended up doing research in very broad and interesting areas in the physical sciences."

All in all, the third TSM conference was a fantastic opportunity to share the successes of all CDT students during the 2015-2016 academic year.

# TYC 10<sup>th</sup> Anniversary

**LARS BLUMENTHAL** (Cohort VI) recalls the conference celebrating the 10 year anniversary of the Thomas Young Centre.

The TYC is an umbrella organisation for groups specialised in theory and simulation of materials from four London Colleges: Imperial College, King's College, Queen Mary University London and University College London. By organising seminars, workshops and many other events, the TYC ensures a regular and stimulating exchange between around 100 research groups from the above institutions to tackle materials problems that are important to industry and society.

Its name is a tribute to Thomas Young (1773-1829) who worked as both a physicist and a physician in London. In his speech after the conference dinner, Dr Andrew Robinson, the author of "Thomas Young: The Last Man Who Knew Everything", highlighted how very broad Young's research interest was. I was surprised to learn that Young studied, amongst other things, light, materials mechanics and surface tension. He is the inventor of the famous double slit experiment and lent his name to the elastic modulus a.k.a. Young's modulus.



**Prof. Giulia Galli captivating the TYC**

To celebrate the 10<sup>th</sup> anniversary of the foundation of the TYC and to showcase that the research conducted by its members and collaborators is at least as versatile as that by Thomas Young himself, the Frontiers of Materials Modelling Symposium was held in London in February. It brought to-

gether an excellent line up of international speakers, all experts in their fields within theory and simulation of materials, and others of the TYC community. Indeed, the interest in this gathering was so large that the organisers struggled to find a big enough venue.



**Interesting discussions continued throughout the conference dinner**

During the first two days of the symposium, we had the pleasure to listen to some excellent talks, which put the current state of TSM in a wider context. The presentations covered a wide range of topics from "soft matter" or "everything you can't take on a plane" (Prof Daan Frenkel, Cambridge), through biological simulations (Prof Mark Sansom, Oxford) to a discussion of cutting edge electronic structure methods (Prof Nicola Marzari, EPFL). I particularly enjoyed Prof Nicola Spaldin's (ETH Zurich) talk discussing the link between perovskite oxides and cosmology since it was a great example of how there is overlap and room for collaboration in even the seemingly most unrelated areas of science. The second night ended with a poster session packed with some of the best science being performed within TSM and the TYC.

On the third and final day the TYC group leaders and industrial collaborators met to discuss the future of theory and simulation of materials and to develop a Roadmap of Materials Modelling to highlight the most important challenges in this field over the next 10-20 years. Keep an eye out for this Roadmap (due to be published soon) to find out how the TYC is set to develop in the coming years.

# TSM Travels the World

The CDT provides a generous annual budget for all students to attend conferences and workshops around the world and meet other scientists working in their field. Here are some of the places TSM students have visited in the last year:



Source: Al MacDonald  
commons.wikimedia.org

## **Dislocations 2016,** West-Lafayette, IN, Nov 2015 **Jonas Verschueren (Cohort VI)**

After a fruitful conference I took a short holiday to Chicago, which is where I took the best pictures. If you want to know what Indiana looks like I suggest you Google 'never ending cornfields'.



Source: C. Ablitt

**A very white White House**

## **APS Division of Fluid Dynamics,** Boston, MA, Nov 2015

### **Freda Jaeger (Cohort V)**

Fluids 2015 was amazing. Mostly because there are lots of pretty simulations and pictures of fluid flows and droplets (plus I got to go to Boston and I loved it).



Source: F. Jaeger

**Overlooking Boston from  
the MIT side**

## **Conference of the American Physical Society,** Baltimore, MD, Mar 2016 **Nicola Molinari (Cohort V)**

APS is a massive conference and not specialised, hence it presents the opportunity to meet great researchers in your field, whilst still having the chance to attend "exotic" talks about aspects of physics that - you think - are unrelated to your PhD. I can always find inspiration from talks, even if they have little in common with my research.

## **Ferro2016,** Washington DC, Jan 2016 **Chris Ablitt (Cohort VI)**

As quite a specialist conference, it was a great place to hear from world experts about cutting edge research in the field of ferroelectrics. I learned a lot from chatting with people who worked on topics very close to my own - and from those who didn't!



### **CECAM Workshop - Interface processes in photochemical water splitting,**

EPFL Lausanne, Switzerland, Sep 2016

**Lars Blumenthal (Cohort VI)**

It was a great workshop as there was an open discussion every day and there was a good mix of leading theorists and experimentalists.

### **GRC Electronic Processes in Organic Semiconductors,**

Tuscany, Italy, Jun 2016

**Alise Virbule (Cohort VI) and Beth Rice (Cohort V)**

Great talks from leading scientists in the field, who we could chat to in an informal setting over dinner whilst eating delicious Italian food.



### **Psi-k Conference,**

San Sebastian, Spain, Sep 2015

**Amanda Diez (Cohort V)**

The entire community of electronic scale simulations was gathered. There were a lot of people from Imperial, the CDT and my office, and it was a great bonding experience, which allowed us to get to know each other better. I remember it was then that I properly met people from Cohort VI that would later join my office in October. The location was fantastic (both the city and the conference centre, which was right next to the beach!). Despite one or two rainy days, the weather was good and allowed us to explore the area!

### **CECAM Workshop - Computational insight into photo-induced processes at interfaces,**

Bremen, Germany, Oct 2016

**Lars Blumenthal (Cohort VI)**

Despite the talks being of really excellent quality, the highlight was, without any doubt, the conference dinner at Jürgenshof.



### **Perovskite Solar Cells and Optoelectronics,**

Genova, Italy 2016

**Andrew McMahon (Cohort V)**

My first time in Italy, and the food was unbelievable. As it is one of the key conferences in my research area, it was great to catch up with collaborators and find out what everyone is up to in the field. It was a good opportunity for networking and people seemed really interested in my work (including an associate editor at a really good journal, who wanted me to send them a draft of my paper!).

# The TSM Family

**DREW PEARCE** (Cohort V) recalls his experiences of the TSM social calendar as he enters his final year in the CDT.

Sometimes it can be hard to remember that life is about more than a PhD and this is where the CDT comes into its own. After I leave, when I will look back at my time at the CDT, my fondest memory will be of the friends I've made along the way.



From the very start there was a calendar packed full of events, which helped us to get to know the welcoming community that TSM is. The first CDT-wide event we were part of was the Christmas Party, which my cohort had to organise when we were in our first year. For me this meant writing the crucially important quiz. This can get very competitive and you must look out for Arash's team who are often the team to beat (or be in!). I really enjoyed developing a fun and (hopefully) unGoogleable quiz.

From then on we've kept a close relationship with our whole cohort, having regular lunches together - something we continued to do throughout our time at Imperial. I've found the cohort really key in building a support network which helps us get through the technical and emotional challenges of a PhD. And the odd free lunch doesn't hurt.



Another important event in the TSM social calendar is the summer BBQ, where, if you are so inclined, you can partake in a bit of light football or rounders. This is a great opportunity to celebrate the rare spells of sunshine London has and also include the CDT's summer students in our community. Mingling with older students and staff is also great for getting an idea for the sort of opportunities available to you as you progress.

Overall, the CDT offers something that non-CDT PhDs don't, a family.

Some example questions from the 'unGoogleable Quiz'. The following mathematical equations represent famous films. See if you can guess what they are:

a)  $\frac{1}{N} \sum_{i=1}^N \left( \text{girl icon} \right)$

b)  $\left[ \text{E} \right] \left[ \text{France} \right] \in \left\{ \text{Earth} \right\} \left( \text{France} \right) \left( \text{Elderly man icon} \right)$

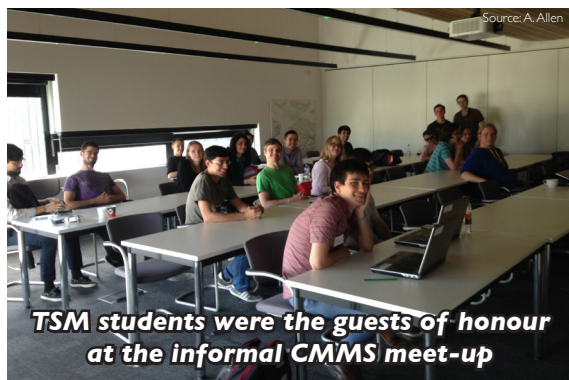
Answers: a) Mean Girls b) No Country for Old Men



# Computational CDT Collaboration

**JONAS VERSCHUEREN** (Cohort VI) on collaborating with the CMMS CDT in Cambridge.

Two years ago the first cohort of students started at the, then newly founded, CDT in Computational Methods for Materials Science (CMMS) in Cambridge. As their projects developed, they fell into the habit of having regular informal meet-ups to present and discuss their work with students of all cohorts. Given the significant overlap of scientific interests between the TSM and CMMS CDTs, we were invited over on the 8<sup>th</sup> of July to one of these meetings, followed by a summery BBQ.



Encouragingly, there was a strong TSM presence on the day and the responsibility of giving talks was divided almost equally between the two centres. Stepping up from the TSM were Chris and Vadim from Cohort V with talks on granular materials and atomistic potentials respectively. Cohort VI was represented by Lars and myself, presenting our respective research in materials for water splitting and high-velocity dislocation mobility. The excellent TSM efforts were matched firstly by Kevin and Alice from

the CMMS who shared their ONETEP projects - on the development and uses in biochemistry respectively - with the group. Finally, Verena discussed the uses of quantum Monte-Carlo methods to study atom-scale many-body interactions. Over lunch a fruitful poster session gave an opportunity to the CMMS masters students to present their research.

From the onset the organisers emphasised that getting to know each other was as important as sharing our research given the similarities between the two CDTs. This was definitely achieved, especially at the BBQ that finished the day off beautifully!

Will this relationship between like-minded CDTs continue? Will this successful meet-up get a return event at Imperial? I definitely hope so but I guess we'll have to wait and see...



# Science & Science Fiction

**ALISE VIRBULE** (Cohort VI) recalls the CDT Festival of Science and Engineering.

The CDT Festival of Science and Engineering is an annual student-led event at Imperial College, mainly aimed at post-graduate students and staff; giving them an opportunity to take a break from day-to-day work and think about science in a different context. This year's theme was "Science and Science Fiction".

Within this theme we aimed to explore the role scientific research plays in science fiction, and vice versa. The core of the programme consisted of talks by speakers from a variety of backgrounds, ranging from a discussion on science fiction and transhumanism by Dr Anders Sandberg (Future of Humanity Institute, University of Oxford) to Mike Mulholland's (Industrial Light & Magic, London) presentation on how high performance computing is used to bring CGI characters to life in the most recent Star Wars films. A definite highlight was the panel discussion on Robotics and Artificial Intelligence (AI) with experts including Shane Legg from Google DeepMind, which was topical since their AI, AlphaGo, had recently beaten the Go world champion Lee Sedol.



Source: A. Rafique

**The organising committee getting excited a day before the festival**

As well as providing great talks, the festival gave attendees the chance to try some hands-on futuristic activities. To complement Emily Smith's and Mike Davis's talk on virtual reality, we brought along several Google Cardboards, which people could use with their own smartphones to experience a simplistic, yet none the less very impressive, virtual reality experience. Additionally, participants tried using their mind to move a cube in 3D space on a screen using an Emotiv EPOC EEG device.



**Preparing to move a cube with her mind**

The organising committee consisted of PhD students from across all the 12 CDTs at Imperial, who had little to no experience in event organisation, so we had to be quick learners to build up an event like this from scratch in just under 4 months. My proudest moment was successfully organising two live Skype talks in a row including a Q&A with an audience of about 150 people.

All in all, overseeing the organisation of an event from the first brainstorming session through to chatting to happy, satisfied guests afterwards was a very valuable experience. I am very much looking forward to attending the festival as a participant next year!

# Taking Science to Pubs

**CHRIS ABLITT** and **ROB CHARLTON** (Cohort VI) tell the story behind *Pint of Science 2016*.

For three nights every May, science takes over local pubs in cities all across the world. Started initially by researchers at Imperial, the Pint of Science festival aims to get the general public engaged in science with the help of world-class speakers, and a couple of pints.

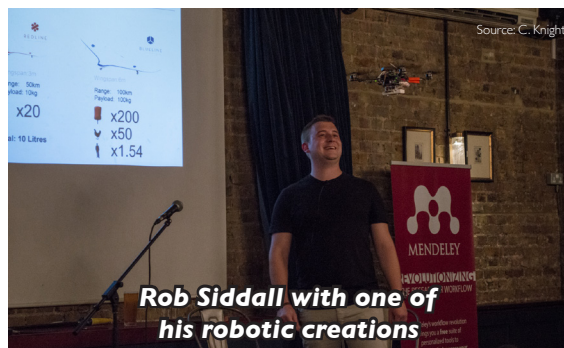
As has become tradition, TSM students once again took up the baton to organise the Imperial College Atoms to Galaxies events. This year, the duty fell to a Gang of Four from Cohort VI to build on the success of previous years. We took over the Boston Room of the George IV in Chiswick, a venue with twice the capacity of any prior Imperial Pint of Science pub. This meant that the pressure was on to live up to high expectations.

Taking the title 'Atoms to Galaxies' quite literally, we chose speakers who provided a perspective of scientific research from many different length and time scales, a theme certainly in keeping with the remit of our CDT! From quantum gravity to dark matter via blast injury, there was something to cater for all tastes at the George IV.



**Prof Johnjoe McFadden putting the pint (and science) in Pint of Science**

The talks were as different in style as they were in content: Dr Emily Mayhew mesmerised the audience as she spoke about the effects of invisible shock waves on the human body while Prof Johnjoe McFadden (University of Surrey) elucidated the origins of life using a pint of Guinness. For us though, the coup de théâtre was when PhD student Rob Siddall used a drone to “deliver” medical supplies over the audience's heads.



**Rob Siddall with one of his robotic creations**

CDT Pint of Science events are notorious for providing hands-on demonstrations courtesy of DrFozzy (CDT Outreach Officer Dr Simon Foster). This year was no exception, with experiments tailored for every talk to bring the science to life, such as creating a cosmic ray detector in a pint glass accompanying Dr Pat Scott's talk on dark matter. Each evening was then topped off with a fiendish quiz as audience members grappled to separate science truth from science fact in a bid to win the coveted Pint of Science pint glass!

After three packed nights of pub science, leaving hordes of happy punters vowing to return next year, we think it's safe to declare Pint of Science 2016 a success. None of this would have been possible without the enthusiastic help of volunteers from across the CDT. No doubt next year will be even better!

# Hermes Summer School

**MITESH PATEL** (Cohort V) describes the two-year long journey of organising Hermes 2016.

When Hermes 2016 took place at Cumberland Lodge, it marked the culmination of two years of hard work for a group of ambitious PhD students who wanted to share their passion for materials modelling and science communication. The members of this group – the Hermes 2016 organising committee – were participants at the previous conference Hermes 2014, and their motivation was to develop upon the legacy of the original event Hermes 2012 over four years ago.

The committee was led by Drew Pearce (Cohort V) and divided into four main sub-committees that respectively handled funding, media, participants and speakers. As Hermes is entirely student-led, the funding team searched for financial means to ensure the event was feasible. The media team campaigned to advertise as far and wide as possible and, through these publicity efforts, the participants team ensured that attendance involved students from a diversity of academic and cultural backgrounds, which is the most important aspect of the school. Finally, the speakers team attracted some world-re-

nowned academics and leading scholars, such as Prof Kurt Kremer (Max Planck Institute for Polymer Research), to deliver exceptional masterclasses about their research.

Along the journey from inception to realisation, we encountered a myriad of challenges from securing funding to promoting the conference. As I was overseeing the speaker sub-committee, the most notable stress-raiser was the event itself - one of our speakers missed their flight the day before their masterclass! Fortunately everything worked out in the end, but participants were absolutely unaware of the commotion and the contingency plan we put into action. It was an invaluable test of character. We learnt much about structuring such an event, but mostly we learnt about ourselves and each other.

Finally, it was an honour to organise such a wonderful event and I hope most of the committee agrees with me when I say that the emotional rollercoaster was totally worth the reward! As we pass on the torch into the very capable hands of Nikoletta Prastiti (Cohort VII) and her team, we wish them good fortune in the wars to come leading up to Hermes 2018, which I am sure will be an amazing event.



Source: D. Spathara

**A happy organising committee at the end of a successful summer school**



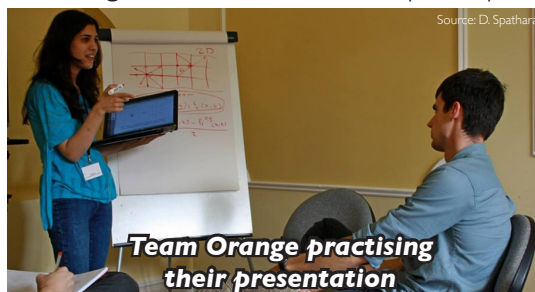
**NIKOLETTA PRASITTI** (Cohort VII) recalls attending the Hermes Summer School.

This year I had the fantastic opportunity to participate in Hermes 2016, which is an interdisciplinary summer school featuring world renowned academics who deliver a series of engaging talks and innovative masterclasses to postgraduate students. The school took place at Cumberland Lodge, which is located outside busy London in a magnificent area full of green and beauty.

The main focus of Hermes is to further stimulate the interest of PhD students in different areas of research across materials science, enhance their science communication skills and develop lasting relationships. The duration of the summer school was only four days (unfortunately). On the arrival day we met our roommates, most of whom came from different colleges and backgrounds. Later that evening, we had an “ice-breaker” challenge where we were divided into groups for a treasure hunt around Cumberland Lodge. This gave us the opportunity to explore the area we were staying in and take breathtaking photos of the spectacular scenery.

The following days were filled with masterclasses in various length scales of materials modelling, ranging from quantum mechanical (Prof Nicola Spaldin, ETH Zurich) up to continuum (Dr Soraia Pimenta, Imperial), as well as technical workshops in Mathematica (Prof Craig Carter, MIT), data visualisation (Lulu Pinney, Freelance Infographer) and presenta-

tion skills (Piero Vitelli, island41). All of these sessions included time for working in teams on a task related to what we’ve learned. Undoubtedly, this boosted our teamwork skills and brought us closer with all the participants.



Source: D. Spatharis

**Team Orange practising their presentation**

On the last day we gave a presentation on a topic we worked on with our teams during the previous days. We chose Lattice Boltzmann dynamics which had been earlier presented by Prof Sauro Succi (Istituto per le Applicazioni del Calcolo). As well as learning in more depth about the method, this task was really a chance to demonstrate the science communication and data visualisation skills acquired through the workshops.

Overall, Hermes proved to be one of the best personal development events I have ever attended. Besides the academic skills I acquired, I have also made lots of friends from different academic backgrounds with whom I will stay connected in the future. I definitely recommend this experience to any student.

Finally, we were so thrilled by this incredible event that we were lead to create a team of volunteers and initiate the procedures for organising Hermes 2018. We are very much looking forward to it!

# Raspberry Pi Cluster

**ADAM READY** (Cohort IV), **MATTHIAS KRAFT** (CMTH) and **FIONN MALONE** (CMTH) recall building a supercomputer from tiny computers.

Any TSM member is acutely aware of the need of large computational clusters and supercomputers, without them a lot of modern research would not be possible. But how about the general public, do they know why the government spends millions of pounds each year to improve computational resources for academics, the MET office, etc.? We thought this would make a great outreach topic, so about a year ago we set out to build a small demo: a 'supercomputer' cluster of ten Raspberry Pis, which combined had 40 cores and 10GB RAM. Not bad considering the low cost!



Building a cluster is relatively easy, but to make the outreach demonstration more exciting and interactive, we decided to use the computers to solve the Tower of Hanoi problem and organised a race between competitive volunteers and either the single or multi-core version of our cluster. Of course even a single core Raspberry Pi is much faster than a human at solving this game, but Dr Simon Foster (CDT Outreach officer) told us not to let the truth get in the way of the story,

so we heavily handicapped the computer so that people could beat the single core time. We used the demo during the physics open day and had prospective students try to beat the machine (one super fast girl even beat the dual core setup).



This was great fun and allowed us to explain to them the ideas and limitations of parallel computing and tell them a bit about our research. As a reward, we had the people with the ten fastest times choose a name for each of the nodes in our cluster:



We hope that the demo could be used at future outreach events such as the Imperial Festival and since all of us are graduating soon, we are looking for volunteers to carry on with the project!



# Ventures beyond the CDT

## Peace Week - From Conflicts to Positive Change

In recognition of the UN Peace Day 2015 **Marise Westbrook** (Cohort VI) gathered a team of ten people to organise a 'Peace Week' with Junior Chamber International London. The half-day Peace Conference featured high-profile speakers, who sparked a lively discussion about local peacebuilding initiatives. Further highlights were a workshop on 'systemic leadership', offering advice on how best to handle personal conflict. The project continues, with an ever-growing team and the 2016 Peace Conference sold out well in advance.



## TSM app to get rail services back on track

Each year over 150 million passenger journeys are delayed in the UK. This summer, TSM student **Ben Kaube** (Cohort III) decided to take a break from writing up his PhD to do something about it. Ben founded social enterprise TrainTrick to help passengers hold train companies to account for delayed and cancelled services. Since launching in July 2016, TrainTrick has been featured on radio, TV and in national newspapers. The Guardian voted TrainTrick as a top 10 travel app alongside Uber and CityMapper.

**The outreach ventures don't stop there** as Mitesh (Cohort V) spent 2 weeks in the Caribbean, visiting remote plantation settlements and helping a doctor in her community healthcare rotation. Beth (Cohort V) runs a weekly science club in Brixton for girls aged 6-10 and has led countless sessions since setting it up in 2013. Vadim (Cohort V) has held several day long workshops for secondary school children, consisting of talks and hands-on activities. Hikmat (Cohort VI) assists in weekly Maths classes at a children's hospital as part of Imperial's Schools Plus programme which aims to inspire and support disadvantaged pupils at local schools. Peter (Cohort V) has written and performed PhysiComedy, a series of free podcasts featuring physics-themed comedy sketches for download ([soundcloud.com/physicomeddy](http://soundcloud.com/physicomeddy)).

**It's not all work and no play** for TSM students as many have talents outside the CDT. To list a few, Andrew (Cohort VII) and Jonas (Cohort VI) play the violin, while Alise (Cohort VI) sings in a choir. On the sportsfield, Freda (Cohort V) plays rugby and Hikmat, Eduardo (Cohort VI) and Chris (Cohort VII), football. Don't mess with TSM students as Gleb, Iacopo, Rob (Cohort VI), Andrew and Mariana (Cohort VII) all practice martial arts!



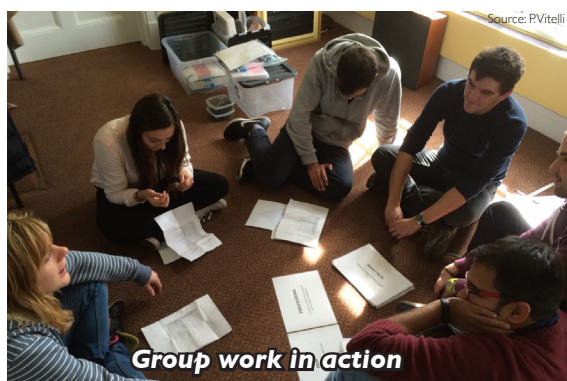
# Authenticity

## **EDUARDO RAMOS FERNÁNDEZ**

*(Cohort VI) recounts his experience at the residential course Authenticity.*

Authenticity is a word created by Piero Vitelli (island41), but if you don't already know what it means, you'll have to wait to find out. It is also the name of a transferable skills course that has been taking place annually since 2011 at Cumberland Lodge whose aim is to provide training on communication, teamwork, networking and presentation skills. Members of Cohort VI were delighted to attend this course in March, mingling with other post-graduate students who had traveled from Bristol, Manchester and Sheffield universities.

The course consisted of a combination of interactive master classes and group activities. The opening session was a "warm up" exercise where we introduced ourselves to each other with the excuse of talking about our PhD projects. We were then split into our groups for the week, formed of people from a mix of universities. A mentor was assigned to each group and we were then asked to write down what we expected from the course as well as the kind of feedback we wanted to receive, which turned out to be one of the most useful outcomes of Authenticity.



The groups worked together to produce a video proposing a solution to a challenge in the modern world (material waste, food waste, education, etc.), along with a five minute presentation that was delivered on the last day of the course. This particular activity encouraged us to work as a team under pressure and time constraints, so the best (and the worst) from us could come out. At the end we had to give and receive individual, constructive feedback to and from each group member.



We also enjoyed several outdoor and indoor group challenges which were both demanding and fun at the same time. Additionally, several presentations on effective networking and teamwork were delivered by experts in those fields, who gave us some useful advice that we had the opportunity to put into practice in other tasks. The course culminated with "Potential Energy", a really engaging talk by Piero about how an outstanding presentation should be delivered, which has definitely changed the way that most, if not all of us, approach public speaking.

To sum up, not only did we meet new people and receive valuable training in non-academic skills, we also got to know ourselves a little better. Having the chance to spot potentially harmful aspects of our behavior when working in teams was priceless. Overall we felt that it was a fantastic and rewarding experience!

# Career Planning Course

**VADIM NEMYTOV** (Cohort V) shares what he learnt at the CDT's annual Career Planning Course.

Prof Adrian Sutton FRS, the founder of our CDT and this careers course, opened the day with a hands-on task to perform a back-of-the-envelope calculation to estimate the odds of becoming an academic in the UK. Considering factors such as the number of PhD graduates each year, the number of faculty positions in the UK, and reasonable assumptions of their age distribution and retirement rate, we finally came up with an estimate. A UK Physics PhD graduate has about a 2-3% chance of getting a faculty position within three years of submitting his or her thesis. Just as Adrian read out this figure thunder struck amidst the heavy rain in Great Windsor Park - or at least so it settled in my memory.



Adrian had set the tone for the course: there is a multitude of rewarding careers beyond academia that one can pursue after obtaining a degree from the TSM. To prove this, he brought along an all-star line-up of worldly scientists. The dream team consisted of a Google product development manager, an

Element Six experimentalist, a science journalist, a science policy maker, an IBM "big data" analyst and, last but not least, a newly minted lecturer at our own department at Imperial: fellowship recipient Dr Johannes Lischner.

I felt that the most valuable experience was to finally lift the veil of mystery and find out what it is that scientists outside the Ivory Tower actually do in their daily jobs. For example, at Element Six, approximately 80% of the workload is experimental: manufacturing artificial diamonds and further optimising this process. Meanwhile, Jassel of IBM explained how they use "tools", such as principal value decomposition and machine learning, to process their clients' data and dig up something useful. All this took place in an informal setting - in small groups we could spend about half an hour with each of the invited guests and ask all and everything. This format was a first for our cohort, and I think most people really appreciated it. Alas, this course is more rewarding the less you know - so I don't want to give away too much. Instead I urge you to sign up for the course yourself!

Overall, the event was certainly useful, even though we all brush shoulders at the TSM, so we had already learnt a thing or two from more senior students and academics - especially about the academic route. The greatest insight came from those who do science in industry describing their day-to-day tasks. The feedback on CVs and cover letters and the workshop on the strategy of building a career were also helpful. All in all, it was a pleasure to spend time with all the participants and speakers at the beautiful Cumberland Lodge, chatting about anything and everything.

# Bosch Masterclass

**NICOLA MOLINARI** (Cohort V) recounts the Masterclass whilst working at Bosch.

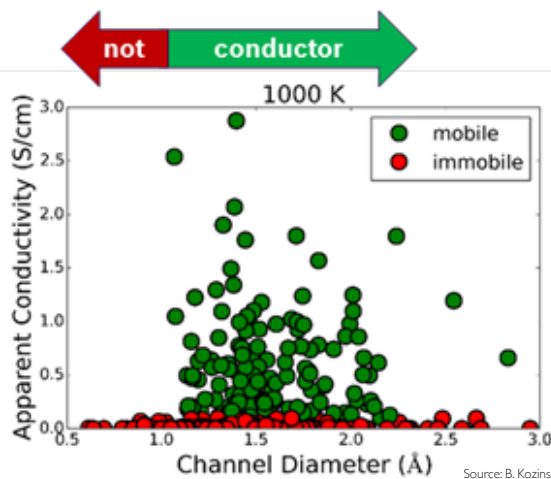
As theoretical/computational PhD candidates are mainly focused on problems that have a tangible connection with reality, what lies beyond the walls of industrial research is of particular interest for TSM students, yet not well understood and sometimes even feared. By speaking with colleagues, the crucial point is whether the industrial environment would force a young researcher to investigate boring, short-term, far from fundamental problems or not. With the aim of shining some light on this topic, in February we had the pleasure of welcoming Dr Boris Kozinsky in our Whiteley HQ for the annual Materials Challenge Masterclass.



After completing his PhD at MIT, Dr Kozinsky was selected to found and lead the Cambridge (MA) Bosch research office. He is currently a Senior Expert at Bosch Research and Technology Center North America, working on next-generation batteries: a topic which is both exciting and important.

During the first hour of the Masterclass, Dr Kozinsky surprised us with a presentation on the work that, along with his team in Cambridge, he had been involved in over the past few years; including a project on thermoelec-

trics, which are materials in which a temperature gradient creates an electric potential. Slide after slide, the audience was surprised by the fact that, whilst maintaining the business and result-oriented approach typical of the industrial sector, the research performed was deeply fundamental, cutting-edge and of real impact.



This figure illustrates an example of an easily computable descriptor (channel diameter in a crystal) that can be used to screen many materials for ionic conductivity.

The curiosity translated into a busy Q&A session. The formality of the Masterclass decreased since the academic staff left and the students had a chance to freely interrogate our speaker about his experience, motivation, ambition and limitations of the industrial research environment. The discussion was followed by a dinner in a local pub between Dr Kozinsky and 20 lucky TSM students.

Personally, I feel that the Masterclass was both interesting and insightful. Our speaker's experience helped us to reconsider some stereotypes we had formed about industrial research and to think about a research position in industry more critically.

# A Shazam Summer as a Service Engineer

**FREDA JAEGER** (*Cohort V*) describes her experience working amongst engineers at Shazam during a summer internship.

Despite the fact that I'm a very proud physicist and have rejected the 'engineer' label many times, I decided to spend my summer among real life engineers. Service engineers, to be precise. For those of you who don't know what that means, don't worry, neither did I when I applied for my internship with Shazam. I fulfilled the requirement of basic Linux knowledge (though none of the others), so I thought I'd give it a shot. And so my internship at Shazam began.

So what is service engineering? Service engineers do anything from system administration and automating deployments of the app to meaningful data extraction. I was on the infrastructure sub team, which meant that my boss and I helped provide and take care of the many servers Shazam uses for both internal and external services. Additionally, I performed statistical analysis on some of

the many, many terabytes of data that they collect. It was particularly interesting to use app store reviews to detect when there are problems with the app and to create methods that flag up when people try to hack the Shazam charts.

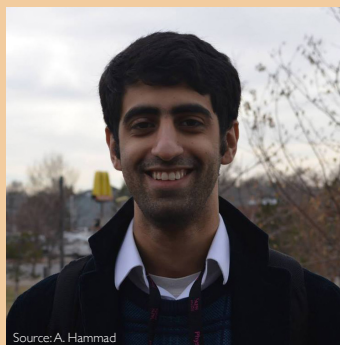


As the UK's flagship tech company, Shazam not only works hard but plays hard too. I much enjoyed the summer party, artist performances, free bagels and lunch and numerous trips to the pub with my colleagues. It is a great place to work since everyone stands behind the product regardless of which part of it they're involved in. And as my boss likes to say, it's good to know that you can "pick up a physicist off the street" (or from Imperial) and they can learn to be a service engineer in just a few months.



# Graduate Spotlights

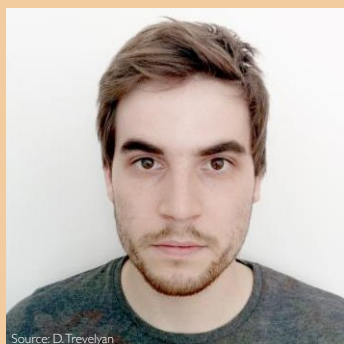
## **DR ALI HAMMAD (COHORT III)**



Source: A. Hammad

I have recently joined the Institute for Infrastructure and Environment, University of Edinburgh as Research Associate in Paste Rheology and Extrusion Simulation. The aim is to conduct fundamental research on the mechanics of granular materials and their interaction with industrial infrastructure, with broad applications in bulk solids handling, paste rheology and fluidisation. The TSM-CDT developed my interdisciplinary theoretical understanding as well as computational skills to prepare me for this post. The programme also enabled me to interact with a diverse group of scientists at different levels of their academic careers which enhanced my understanding of the many ways in which science can contribute towards real life problems. These problems could range from particle to full-industrial scales, and from dry to multiphase systems. Novel discrete and continuum theories, numerical methods and experimental techniques are being developed to enable such research.

## **DR DAVID TREVELYAN (COHORT II)**



Source: D. Trevelyan

At Jukedeck, we're building an artificially-intelligent music composer, performer and producer. I'm responsible for building a suite of tools that automatically converts composed musical scores into a coherent piece of digital audio. I encounter new problems every day that require an advanced knowledge of computational mathematics in a diverse set of disciplines that range from complex analysis in digital signal processing to statistics in machine learning. I was fortunate that the MSc part of the TSM-CDT gave me the mathematical foundation necessary to truly understand these problems, and the PhD years gave me the freedom to really explore modern best-practice computer programming. The most profound influence that the TSM-CDT had on me was seeing the value placed on interdisciplinary research; solutions to problems are easier to find when you have a broader knowledge and access to a fresh perspective.

# Where a PhD in TSM can take you

**DR RICHARD BROADBENT (COHORT I)**

Lifing Technologist  
Rolls-Royce

**DR DAVID EDMUNDS (COHORT I)**

Postdoctoral Research Fellow  
The Royal Marsden NHS Trust

**DR JOE FALLON (COHORT I)**

Data Analyst  
Government Operational Research Service

**DR ROBERT HORTON (COHORT I)**

Quantitative Analyst  
Principal Global Investors

**DR JASSEL MAJEVADIA (COHORT I)**

Data Scientist  
IBM

**DR AENEAS WIENER (COHORT I)**

CTO and Founder  
Cytora

**DR ANTHONY LIM (COHORT II)**

Research Fellow  
University College London

**DR JAWAD ALSAEI (COHORT II)**

Assistant Professor  
University of Bahrain

**DR NICCOLO CORSINI (COHORT II)**

Founder  
Sonodot

**DR BEÑAT GURRUTXAGA-LERMA (COHORT II)**

Junior Research Fellow  
University of Cambridge

**DR FABIAN RENN (COHORT II)**

Senior Software Engineer  
ROLI

**DR THOMAS SWINBURNE (COHORT II)**

Research Fellow  
Culham Centre for Fusion Energy

**DR JOSHUA TSANG (COHORT II)**

Secondary School Teacher  
Hammersmith Academy

**DR THOMAS POOLE (COHORT II)**

Senior Software Engineer  
ROLI

**DR VALERIE VAISSIER (COHORT II)**

Postdoctoral Scholar  
UC Berkeley and LBNL

**DR TIM ZUEHLSDORFF (COHORT II)**

Postdoctoral Scholar  
University of California Merced

**DR MARC COURY (COHORT III)**

Graduate Software Engineer  
BAE Systems Applied Intelligence

**DR THOMAS EDWARDS (COHORT III)**

Software Engineer  
First Light Fusion

**DR DANIEL RATHBONE (COHORT III)**

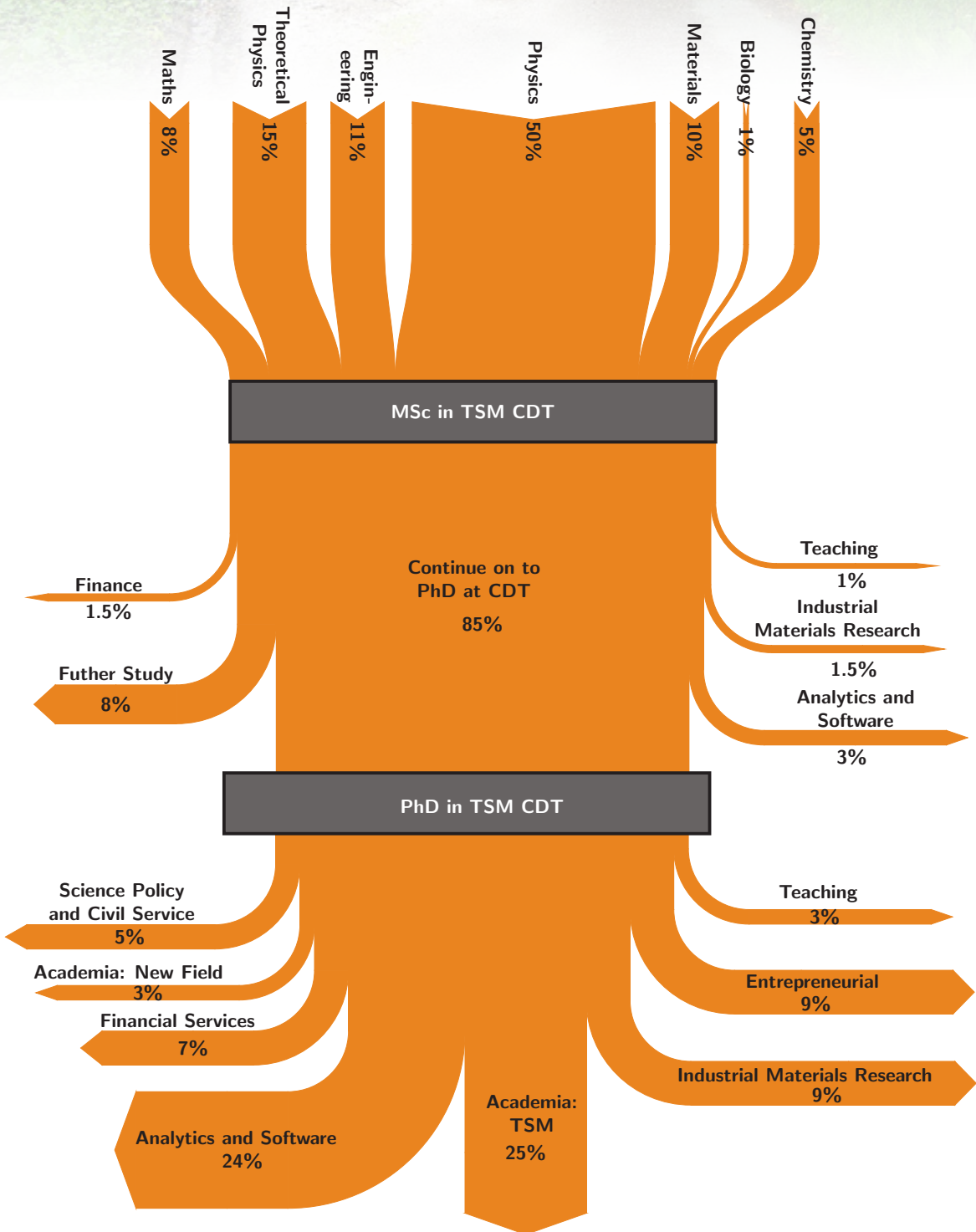
Research Analyst  
House of Commons

**DR CHRISTOPHER ROCHESTER (COHORT III)**

Quantitative Analyst  
PrismFP

*Disclaimer: This list was compiled using linkedin and institutions' websites as sources, therefore we can't guarantee that the information is up-to-date.*

# Origins and Destinations





# Selected Student Publications

**A Molecular Model For HNBR With Tunable Cross-Link Density** - **N. Molinari, M. Khawaja**, A. P. Sutton and A. A. Mostofi, J. Phys. Chem. B, accepted (2016)

**Efficient simulations with electronic open boundaries** - A. P. Horsfield, **M. Boleininger**, R. D'Agosta, V. Iyer, A. Thong, T. N., and C. White, Phys. Rev. B, 94 (7), 075118, Aug 2016

**Charging ultrananoporous electrodes with size-asymmetric ions assisted by apolar solvent** - **C. C. Rochester**, S. Kondrat, G. Pruessner and A. A. Kornyshev, J. Phys. Chem. C, 120 (29), 16042, Jul 2016

**Fluctuating-bias controlled electron transport in molecular junctions** - **M. Ridley**, A. MacKinnon and L. Kantorovich, Phys. Rev. B, 93 (20), 205408, May 2016

**A numerical study exploring the effect of particle properties on the fluidisation of adhesive particles** - **R. Wilson**, D. Dini and B. van Wachem, Aiche Journal, 62, (5), 1467, May 2016

**Hubbard-like Hamiltonians for interacting electrons in s, p, and d orbitals** - **M. E. A. Coury**, S. L. Dudarev, W. M. C. Foulkes, A. P. Horsfield, Pui-Wai Ma, and J. S. Spencer, Physical Review B 93, 075101, Feb 2016

**Free-energy coarse-grained potential for C60** - **D. Edmunds**, P. Tangney, D. Vvedensky and M. Foulkes, The Journal of Chemical Physics Vol 143 No 16, Oct 2015

**Pressure-Induced Amorphization and a New High Density Amorphous Metallic Phase in Matrix-Free Ge Nanoparticles** - **N. R. C. Corsini**, Y. Zhang, W. R. Little, A. Karatutlu, O. Ersoy, P. D. Haynes, C. Molteni, N. D. M. Hine, I. Hernandez, J. Gonzalez, F. Rodriguez, V. V. Brazhkin, and A. Sapelkin, Nano Letters, 15 (11), Oct 2015

**Surface morphology of CuFeS<sub>2</sub>: The stability of the polar (112)/ $\overline{(112)}$  surface pair** - **V. H. -Y. Chen**, G. Mallia, R. Martinez-Casado and N. M. Harrison, Phys. Rev. B, 92 (15), 155426, Oct 2015

A comprehensive list of student publications can be found at  
<http://www.imperial.ac.uk/theory-and-simulation-of-materials/research/student-publications/>

## 2016 Awards

**Sutton Prize for the best overall performance in the TSM MSc**  
Maciej Jarocki

**Johnson Matthey PhD prize winner**  
Chris Rochester

# Current Students and Research Projects

## Cohort IV



**Max Boleininger**—*Ultrafast Laser Interactions with Thin Polymer Films (with funding from US Air Force Research Laboratory)*

Dr Andrew Horsfield (Materials), Prof Jonathan Marangos (Physics), Prof Peter Haynes (Physics/Materials), Dr Ruth Pachter (US AFRL)



**Stephen Burrows**—*Lattice Boltzmann Simulation of Complex Fluid Rheology*

Dr Fernando Bresme (Chemistry)



**Andrea Greco**—*Theory and Simulation of Complex Oxide Materials (with funding from Argonne National Lab)*

Dr Arash Mostofi (Physics/Materials), Dr John Freeland (Argonne National Laboratory)



**Chiara Liverani**—*Quantum Effects in Hydrogen Embrittlement*

Prof Mike Finnis (Physics/Materials), Dr Eva-Maria Graefe (Mathematics)



**Adam Ready**—*Why is Ti6242 Susceptible to Cold Dwell Fatigue, but Ti6246 Is Not? (with funding from Rolls-Royce)*

Prof Adrian Sutton (Physics), Prof Peter Haynes (Physics/Materials), Prof David Rugg (Rolls-Royce)



**Michael Ridley**—*Quantum Effects of Electronic Transport on Atomic Dynamics in Molecular Junctions and Organic Semiconductors*

Prof Lev Kantorovich (KCL - Physics), Prof Angus MacKinnon (Physics)



**Mahdiah Tajabadi Ebrahimi**—*Multiscale Investigation of Failure in Bonded Diamond Aggregate (with funding from Element Six)*

Prof Daniele Dini (Mech. Eng.), Dr Daniel Balint (Mech. Eng.), Prof Adrian Sutton (Physics), Dr Serdar Ozbayraktar (Element Six)



**Robert Wilson**—*A Multi-Scale Approach to Understanding Cohesive Particle Flows*

Prof Daniele Dini (Mech. Eng.), Dr Berend Van Wachem (Mech. Eng.), Dr Michele Marigo (Johnson Matthey)

# Cohort V



**Amanda Diez**—*Structures and Processes in a Quantum Rattle*

Prof Mike Finnis (Materials/Physics), Prof Molly Stevens (Materials)



**Peter Fox**—*Nanoplasmonics and Metamaterials at the Classical/Quantum Boundary*

Prof Ortwin Hess (Physics), Prof Stefan Maier (Physics)



**Frederike Jaeger**—*Flow of Fluids Through Disordered Media with Application to Membranes: from the Molecular to the Continuum through the Meso-Scale*

Prof Omar Matar (Chem. Eng.), Prof Erich Muller (Chem. Eng.)



**Chris Knight**—*Multi-Scale Analysis of Liquefaction Phenomena in Soils*

Dr Catherine O'Sullivan (Civ. Eng.), Prof Daniele Dini (Mech. Eng.), Dr Berend Van Wachem (Mech. Eng.)



**Andrew McMahon**—*The Behaviour of Charged Species in Hybrid Organic-Inorganic Perovskite Photovoltaics*

Prof Nicholas M. Harrison (Chemistry), Dr Piers R.F. Barnes (Physics), Prof Joost VandeVondele (ETH Zürich - Materials)



**Nicola Molinari**—*Towards a Predictive Model of Elastomer Materials (with funding from Baker Hughes)*

Dr Arash Mostofi (Materials/Physics), Prof Adrian Sutton (Physics), Dr David Curry (Baker Hughes), Dr John Stevens (Baker Hughes)



**Vadim Nemytov**—*Nanocrystals by Design: Combining the Power of Atomistic Force Fields and Linear-Scaling Density Functional Theory (with Materials Design scholarship)*

Dr Paul Tangney (Materials/Physics), Prof Peter Haynes (Materials/Physics)



**Premyuda Ontawong**—*Atomistic-to-Continuum Theory of Martensitic Transformations*

Prof Dimitri Vvedensky (Physics), Prof Lev Kantorovich (KCL - Physics), Dr Carla Molteni (KCL - Physics)



**Farnaz Ostovari**—*Modelling Damage in Environmental Barrier Coatings on Woven SiC/SiC Composite Substrates*

Dr Daniel Balint (Mech. Eng.), Prof Ferri Aliabadi (Aeronautics)



**Mitesh Patel**—*Multiscale Modelling of Delayed Hydride Cracking (with funding from Rolls-Royce)*

Dr Daniel Balint (Mech. Eng.), Dr Mark Wenman (Materials), Prof Adrian Sutton (Physics)



**Drew Pearce**—*Approaches and Challenges in the Coarse-Graining of Conjugated Molecular Materials.*

Prof Jenny Nelson (Physics)



**Beth Rice**—*Tight-Binding Approach to the Simulations of the Electronic and Optical Properties of Porous Conjugated Molecular Materials*

Prof Jenny Nelson (Physics), Dr Jarvist Moore Frost (Physics), Dr Kim Jelfs (Chemistry)



**Markus Tautschnig**—*Corrosion Scale Dynamics: Towards a Predictive Model for Sweet/Sour Corrosion Scale Formation (with funding from BP)*

Prof Nicholas M. Harrison (Chemistry), Prof Mike Finnis (Materials/Physics)

## Cohort VI



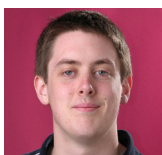
**Chris Ablitt**—*First Principles Lattice Dynamical Study of Ferroelectric and Negative-Thermal-Expansive Ruddlesden-Popper Oxides*

Dr Arash Mostofi (Materials/Physics), Dr Nicholas Bristowe (Materials), Dr Mark Senn (Oxford - Chemistry)



**Lars Blumenthal**—*Electronic Excitations at Solid-Liquid Interfaces: Combining Many-Body Perturbation Theory with Molecular Dynamics Simulations*

Dr Paul Tangney (Materials/Physics), Dr Johannes Lischner (Materials/Physics)



**Robert Charlton**—*Computational Excitonics of Doped Organic Molecular Crystals for a Room Temperature Maser (with an Imperial College PhD Scholarship)*

Prof Peter Haynes (Materials/Physics), Dr Andrew Horsfield (Materials)



**Luca Cimbaro**—*Embrittlement of Ni-based Superalloys by Oxygen (with funding from Rolls-Royce)*

Dr Daniel Balint (Mech. Eng.), Prof Tony Paxton (KCL - Physics), Prof Adrian Sutton (Physics)



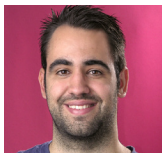
**Jacek Golebiowski**—*Polymeric CNT Composites – Atomistic Simulation of the Effects of CNT Functionalisation on Interfacial Properties (with co-funding from the Marie Skłodowska-Curie European Training Network "TheLink")*

Prof Peter Haynes (Materials), Dr Arash Mostofi (Materials/Physics)



**Hikmatyar Hasan**—*Designing Next Generation High-Temperature Co-Al-W Based Superalloys*

Dr Vassili Vorontsov (Materials), Prof Peter Haynes (Materials/Physics), Prof David Dye (Materials)



**Eduardo Ramos Fernández**—*Multi-Scale Modelling of Hydrodynamic Lubrication and Friction (with funding from BP)*

Prof Daniele Dini (Mech. Eng.), Prof David Heyes (Mech. Eng.)



**Iacopo Rovelli**—*High Temperature Loss of Strength in Ferritic/Martensitic Steels for Fusion Energy Applications (with funding from Culham Centre for Fusion Energy)*

Prof Adrian Sutton (Physics), Prof Sergei Dudarev (Physics)



**Gleb Siroki**—*Optical Properties of Topological Insulator Nanoparticles*

Dr Vincenzo Giannini (Physics), Dr Derek Lee (Physics), Prof Peter Haynes (Materials/Physics)



**Jonas Verschueren**—*Fundamentals of Dislocations in Motion*

Prof Daniele Dini (Mech. Eng.), Dr Daniel Balint (Mech. Eng.), Prof Adrian Sutton (Physics)



**Alise Virbule**—*Design of High Absorption Organic Semiconductors for Applications to Solar Cells and Light Emission*

Prof Jenny Nelson (Physics), Dr Johannes Lischner (Materials/Physics)



**Marise Westbroek**—*Flow in Porous Media (with Janet Watson scholarship)*

Prof Peter King (Earth Sci. and Eng.), Prof Dimitri Vvedensky (Physics)

## Cohort VII



**Fangyuan Gu**—*Controlling structural change in multiferroic materials by ultra-fast laser excitation*

Dr Éamonn Murray (Materials/Physics), Dr Paul Tangney (Materials/Physics)



**Nikoletta Prastiti**—*Development of fracture in weakly consolidated media (with funding from BP)*

Prof Peter King (Earth Sci. and Eng.), Prof Rafi Blumenfeld (Earth Sci. and Eng.)



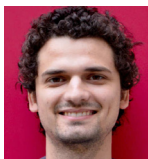
**Lara Román Castellanos**—*Hot electrons in nanoplasmonics: combining quantum mechanics with nanophotonics*

Prof Ortwin Hess (Physics), Dr Johannes Lischner (Materials/Physics)



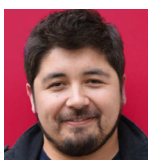
**Andrew Warwick**—*Emergent Phenomena at domain walls in halide perovskites*

Dr Nicholas Bristowe (Materials), Prof Peter Haynes (Materials/Physics)



**Ignacio Bordeu**—*Theory of active matter (with funding from Conicyt)*

Dr Gunnar Pruessner (Mathematics), Prof Henrik Jensen (Mathematics)



**Harry Cárdenas**—*Molecular thermodynamic models for adsorption (with funding from Conicyt)*

Prof Erich A. Müller (Chem. Eng.)



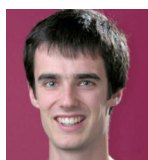
**Mariana Hildebrand**—*Towards the manipulation of defects and dopants to functionalise graphene (with funding from the National Physical Laboratory)*

Prof Nicholas M. Harrison (Chemistry), Prof Peter Haynes (Materials/Physics), Dr Ivan Rungger (NPL)



**Nuttawut Kongsuwan**—*Strong Coupling in Plasmonic Nanocavities (with funding from the Thai Government and Imperial College)*

Prof Ortwin Hess (Physics)



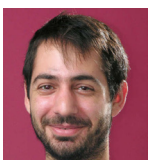
**Charles Penny**—*The contribution of surfaces to the magnetic Curie temperature and magnetic recording fidelity (with funding from STFC)*

Dr Adrian Muxworthy (Earth Sci. and Eng.), Dr Karl Fabian (NGU, Norway) and Prof Valera Shcherbakov (RAS, Russia)



**Christopher Sewell**—*Advancing the atomistic theory of corrosion passivation in sulfidic environments (with funding from BP)*

Prof Nicholas M. Harrison (Chemistry), Dr Paul Tangney (Physics/Materials)



**Panagiotis Simatos**—*The impact of combustion-generated moieties on the degradation of ICE related surface materials (with funding from Toyota Motor Europe)*

Prof R. Peter Lindstedt (Mech. Eng.) , Prof Daniele Dini (Mech. Eng.), Dr Konstantinos Gkagkas (Toyota Motor Europe)

## Cohort VIII — A warm welcome!

**Martik Aghajanian, Cristian Constante Amores (with funding from BP), Sophie Finnigan, Emanuele Galiffi, Syed Hussain, Wuwei Jin, Xiaomin Meng, Samuel Palmer, Angeliki Poulou, Luca Reali, Marie Rider, Jana Smutna, Anthony Spice, Alike-Marina Tsopeleakou (with funding from Toyota Motor Europe), Tomos Wells (with funding from Culham Centre for Fusion Energy)**

# Members of the Advisory Board

## External Advisors

**Dr Anna Angus-Smyth** – EPSRC Representative

**Prof W Craig Carter** – Massachusetts Institute of Technology, USA

**Dr David Curry** – Baker Hughes, UK

**Prof Sergei Dudarev** – Culham Centre for Fusion Energy, UK

**Dr Claire Hinchliffe** – Sheffield-Manchester CDT in Advanced Metallic Systems, UK

**Prof David Rugg** – Rolls-Royce, UK

**Dr Simon Schultz** - CDT in Neurotechnology, ICL, UK

**Prof Helena Van Swygenhoeven** – Paul-Scherrer Institute & EPFL, CH

**Dr Erich Wimmer** – Materials Design, Inc., USA/France

## TSM-CDT Members

**Dr Arash Mostofi** – Director and Cohort IV Mentor

**Dr Johannes Lischner** – Assistant Director

**Prof Peter Haynes** - Strategic Advisory Team

**Prof Adrian Sutton** - Strategic Advisory Team

**Dr Daniel Balint** – Cohort Mentor: Cohort V

**Prof Mike Bearpark** – Cohort Mentor: Cohort VI

**Dr Andrew Horsfield** – Cohort Mentor: Cohort VII

**Dr Kim Jelfs** - Cohort Mentor: Cohort VIII

**Dr Simon Foster** – Outreach Officer

**Ms Miranda Smith** – Senior CDT Administrator

**Ms Veena Dhulipala** - CDT Administrator

For a full list of staff see:

<https://www.imperial.ac.uk/theory-and-simulation-of-materials/people/staff/>

## Contact Details

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