# Annual Report

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


2018

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London, March 2019

*'This wasn't a race. It was a pilgrimage.'*

- Henri Pélissier, 1919

# Contents

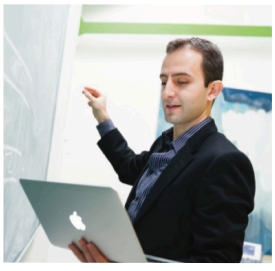
# Director's Foreword

This has been a bitter-sweet year for me and for the Centre for Doctoral Training in Theory and Simulation of Materials (TSM-CDT). The TSM-CDT was founded in 2009 by Professor Adrian Sutton FRS with a mission to create a new generation of scientists and engineers with the theoretical and computational skills to model processes and phenomena in materials across length and time-scales. Adrian sought to address the major problem that theoretical materials science had all but disappeared from undergraduate physics curricula, at the same time that undergraduates of materials science and engineering seldom received rigorous training in the computational and theoretical methods needed to develop predictive, physically-based models of the behaviour of materials. What's more, phenomena in materials at different scales are interconnected, whereas the disciplinary silos in which students are traditionally trained (physics, chemistry, engineering, ...) tend to focus their attention on specific scales and often use different languages to describe the same things.

Adrian, therefore, resolved to create a programme that would take students from different disciplinary backgrounds and provide them with a rigorous, multi-disciplinary education in TSM across length and time-scales. One crisp Autumn morning in 2008, Adrian, Prof Peter Haynes and I went to EPSRC HQ in Swindon to justify to a panel of senior academics why we needed £6.4M (on top of a similar amount of funding from the College and our industry partners), to make this vision a reality through training five cohorts of 10 students each. The panel decided to give us the opportunity and, as they say, the rest is history. In 2014 the TSM-CDT was renewed for a further five cohorts, this time with even greater financial leverage from our industry partners who saw the enormous value in what we were doing: training a pipeline of highly skilled problem-solvers, independent thinkers, and team-players with the confidence to make important contributions in their chosen fields.

All good things, however, come to an end. This year, we welcomed our tenth and final cohort of students to the TSM-CDT. As I reflect on the past ten years, there are many things that have given me great satisfaction and pleasure, but three in particular really stand out. Firstly, the privilege of working with such a great team of academic staff, support staff, students and external partners. Without your support and enthusiasm, the CDT would not have flourished as it has done. Within the pages of this annual report, you will see a small snapshot of what this team is able to achieve. Second, the culture change that the TSM-CDT has catalysed towards multi-disciplinary research, which is evidenced by the remarkable network of cross-disciplinary collaborations that has been generated and which would not have been possible without the CDT. And finally, the quality of our graduates who are already making waves in their careers in industry, technology, consulting, academia and elsewhere. These are the enduring legacies of the TSM-CDT that will continue to resonate long after the final cohort of students graduates.

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



# Going for Gold:
## The Path to a PhD

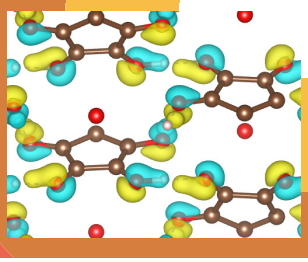

L-R: Cohort lunches, a warm welcome outside Whiteley, and nutrition powers training: enjoying pizza at the MSE Congress trip.

Image credits: D. Ho; M. Smith

## Training Blocks

**Encompassing lecture courses across physics, materials science and computational methods, the Masters year provides the all-important training for PhD victory.**

**Cohort 9 reflect back on their first year with the CDT and how they were prepped with the tools for research success.**



Left: Visualising the difference in electron density between two ferroelectric configurations.

Credit: M. Okenyi

### Matthew Okenyi

Ferroelectrics are a class of materials which produce a spontaneous electric dipole. This occurs because internal charge (due to ions and electrons) is naturally separated in space in these materials. In my project, I am interested in a recently discovered family of organic ferroelectrics. Compared to the traditional inorganic counterparts, organic ferroelectrics could become cheaper, more environmentally friendly alternatives for applications in optics, actuation, memory chips and temperature sensing devices.

In order to understand a ferroelectric, the strength of the interactions between ions in the material have to be calculated. I have found the Electronic Structure of Materials courses in the MSc very useful, since they introduced me to density functional theory (DFT), a formulation of quantum mechanics that allows me to measure these interactions, among other useful quantities.

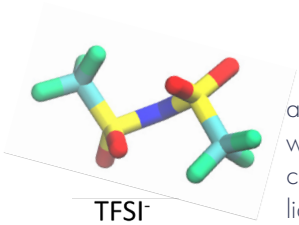
The Methods for Simulation of Materials course was also helpful since it gave me a grounding in molecular dynamics, a method by which the finite-temperature motion and stability of ions about the equilibrium sites predicted by DFT can be quantified.

**Intensive training with a constant chase for progress. A large need for individual motivation, drive and determination. A long term, highly personal goal at the end of 4 years.**

**Without a doubt, if a PhD was an Olympic event it would be the Marathon.**

**Meet some of our Mo Farah members of the CDT as they share experiences from start to finish of the journey to earning 'Dr'.**

## Zachary Goodwin





Room temperature ionic liquids (RTILs) are, in principle, solvent-free electrolytes with melting points below 100°C. Such concentrated electrolytes remain in the liquid phase due to the highly complex shapes and asymmetric sizes of the constituent ions, with cations typically being the bulkier ion. RTILs are rarely solvent free, however, since most are hygroscopic or there is the addition of organic solvents to reduce the viscosity. Hence, it is important to understand the response of solvent-in-RTILs to electrified interfaces. My MSc project aimed to better understand excluded volume and correlation effects in these complex systems through the application of simple, analytical continuum models.

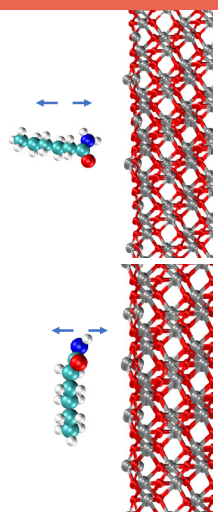
The Equilibrium in Materials courses prepared me for the MSc project well, since we thoroughly covered mean-field continuum models, such as the Langmuir adsorption model. The Computational Methods course also helped to prepare me for the task of solving the highly non-linear modified Poisson-Fermi equation which was derived to describe solvent-in-RTILs at electrified interfaces.

Above: Two constituent ions: trifluoromethanesulfonate (OTF-) and bis(trifluoromethane sulfonyl)imide used in solvent-in-RTIL simulations. (Credit: Z. Goodwin) Right: Selecting talks during the MSc conference trip to the MSE Congress. (Credit: D. Ho)

## Carlos Ayestarán Latorre

Lubricant additives are employed to reduce friction and wear in engines and machinery. Occurring in several shapes and colours, the varied chemical nature of the additives dictates the respective lubricity mechanism. For example, organic friction modifiers (OFMs) adsorb and arrange in closely-packed monolayers that preserve the surface, whereas zinc dialkyldithiophosphates (ZDDP) undergo a chemical reaction due to shear stresses that result in the growth of protective, amorphous tribofilms. The nature of these systems naturally requires bridging first principles and classical simulations. My MSc project involved developing a classical force-field for molecular dynamics (MD) for an OFM from density functional theory (DFT) simulations.

The Methods for Simulating Materials course has definitely been useful for me, as we covered the basics of both MD and DFT. Electronic Structure of Materials was also relevant as it presented the mathematical grounds of DFT itself, extremely necessary in order to avoid using DFT as a physically unmotivated black box. Finally, I have also made valuable use of the tools learned in Computational Methods, especially Python.

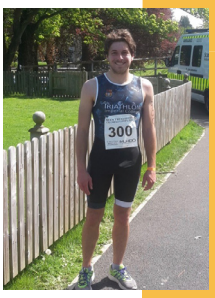


Above: Simulations of an OFM (hexanamide) interacting with an iron oxide surface.

Credit: C. Ayestarán Latorre

# Starting Blocks

**Race time! Initial training complete, Luca Reali looks back at starting the PhD main event with cohort 8**



Above: Maintaining work-life balance. Luca with the volleyball team and ready to tri.

Credit: L. Reali

The majority of TSM-CDT PhDs do not start afresh, but build on top of the Masters year projects, often with a seamless transition involving the same topic and supervisors. This greatly eases the first period. I felt like I just had to carry on with what I had already been doing for months. One becomes more and more expert, perhaps without realising it. Someone once told me: in a few months, you should be understanding more about the specific topic than your supervisors themselves. I am not sure this is quite the case, but it gives the idea of what it means to get up every morning with the same questions (and nightmares!) in mind.

Beyond this transition, there are different ways in which a PhD project can start out and these were encompassed across out cohort. Some people have to 'test the water' in several ponds and go back and forth from one to another, some others just dive into the right one and start swimming like a shark. I definitely fall within the former group: my project started quite slowly. I had to read a lot and convince my supervisors to alter the title and aim, but I now feel more confident. Especially in situations like mine, your supervisor's help is crucial and I am greatly indebted to them.

Outside of work, moving into the PhD gave me more time to explore other aspects of life at Imperial, from returning to playing volleyball to trialling a triathlon.

# Hitting the Wall

**Infamous for motivational droughts and slow progress, the middle years of PhD research can be tough.**

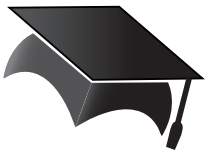
**Nikoletta Prastiti (cohort 7) shares her highs and lows from the second year of her PhD**

Windsor park wildlife: the Hermes organising committee and the local residents strike a pose during Hermes 2018.

Credit: N. Prastiti (top) and S. Finnigan (bottom)

The middle year of the PhD has been quite a challenge.

It mostly involved me revisiting results and analyses from my first year and making important adjustments and improvements. I developed a systematic research methodology which helped me organise the plethora of scientific information I had gathered throughout my first year as a PhD student. I realised the importance of filtering through the relevant information in a scientific report and started storing that information in libraries which I can easily access using keywords.



# Finishing Straight

**Finish line is in sight, Chris Ablitt gives us the cohort 6 lowdown on tackling the final stretch**

"What are you going to do once you graduate?", "you don't have long left of your funding, right?", "have you written that thesis yet?". These are three questions you should never ask a final year PhD student, although it seems like not many people saw that public health announcement. Coming to the end of your PhD is a strange time. Whereas tangents used to be intriguing rabbit holes to explore, once you count the remaining time in months and not years your thoughts instead turn to ways to wrap projects up quickly.

For our cohort, the last six months have been especially strange since most, but not all of us, took time out of our PhDs to undertake internships of varying lengths. This may imply that we're taking forbidden question #1 seriously, but also means that some of the cohort have already entered the Big Wide Scary World of Work. While for others, the thesis remains a document that we probably should have started writing... Although our timelines may have diverged, our sense of cohort community has not – at the time of writing we have just had our final Cohort Lunch (although as firm friends we will continue to meet up without the capital letters). Reflecting back as a TSM-CDT-OAP, I am grateful for the support and community the CDT provided and wouldn't have wanted to do a PhD any other way.

Above right: Cohort 6 enjoy a final cohort Christmas lunch together. (Credit: M. Bearpark) Left three: Graduation celebrations for PhD and MSc TSM-CDT students (Credit: M. Smith)

There were many days where motivation was low. This is normal when you are stuck on the same problem for days (or even weeks!), but I found that taking a break and distancing yourself from the problem for a while, may help you return more motivated and refreshed. In addition, motivation can reignite by discussing your problem with colleagues working on similar questions who could supply new ideas to apply to your own research.

One of the highlights of my second year was attending a conference in New York. I won a prize for the talk that I presented and made important contacts that have led to collaborations. Another highlight was the successful organisation of the Hermes summer school - a 2-year journey full of beautiful memories and soft skills development (discover more on page 16).

Overall, even though the second year has been challenging, I've become a more organised and therefore, a better researcher. Additionaly, I also found that communicating with other people in the field significantly increases motivation and inspiration. I am looking forward to seeing how the final year unfolds.

# Research Highlights

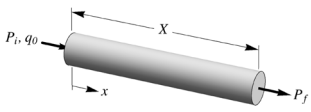
Explore the range of CDT research as we traverse the multi-scale to unlock new simulation secrets, combine the power of light and the nanoscale, and discover the intricacies of navigating from A to B.

## Path Integrals for Darcy Flow

*Marise Westbroek introduces her work on a path integral formulation of flow through porous media*

The path integral method, well known in theoretical physics, is a tool to obtain all accessible information about the position of a quantum particle. Let us suppose the particle was observed at point A at time $t_A$ and then at point B at time $t_B$. Where was the particle in the time interval $t_B - t_A$? By the nature of quantum mechanics, we cannot calculate its path, as we would for a classical particle. There exists a variety of conceivable paths from A to B; some paths are more likely than others.

A path integral is a weighted integral over all possible paths. The smaller the amount of energy the particle needs to traverse a given path, the greater the probability weight attached to that path. The path integral contains the full statistical information about the particle's whereabouts between $t_A$ and $t_B$. To calculate the path integral numerically, possible paths are simulated on a lattice.[1]




A schematic depiction of one-dimensional flow.

We have applied the path integral to the problem of one-dimensional flow through porous media. Examples of flow through a porous medium include the flow of oil through a rock, water infiltration into the soil, the flow of oxygen through lungs and hemodynamics through blood vessels.

In order to study the flow on a large scale, the porous medium is coarse-grained. We do not know the exact structure of the permeability of the medium. However, based on fieldwork, we can make reasonable assumptions about its mathematical nature and describe it in terms of a correlated stochastic process. Given that the pressure can be fixed at $p_A$ at point A and at $p_B$ at point B, we can calculate the integral over the 'pressure paths' (Fig 1) of the fluid, analagous to the one-dimensional example paths below. By calculating the path integral, we can achieve a complete statistical representation of the fluid's pressure between points A and B.

The results of our path integral simulations are in excellent agreement with traditional methods to calculate the flow through a porous material. The details of both calculations can be found in refs 2 and 3. In the future, we look to extend our method to multiphase flow.

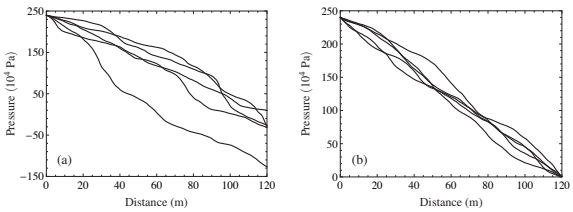


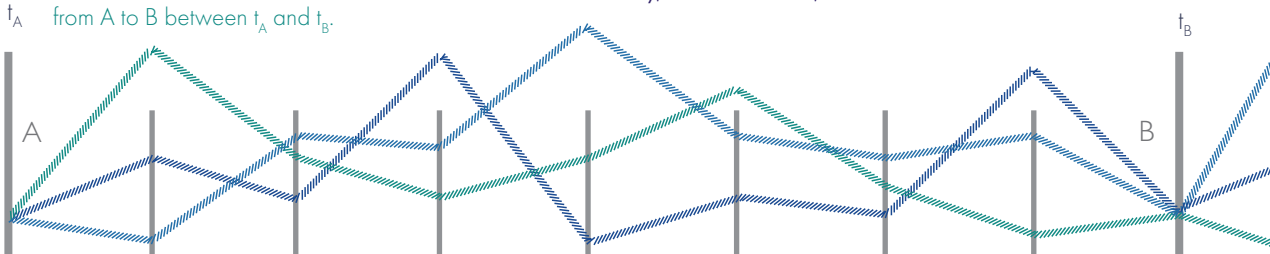

Fig 1: Examples of calculated pressure paths.


1: M. J. E. Westbroek, P. R. King, D. D. Vvedensky and S. Duerr, Am. J. Phys. 86, 293, 2018

2: M. J. E. Westbroek, G.-A. Coche, P. R. King and D. D. Vvedensky, Phys. Rev. E 97, 042119, 2018

3: M. J. E. Westbroek, G.-A. Coche, P. R. King and D. D. Vvedensky, arXiv: 1811.01781, 2018


One dimensional paths can be simulated on a lattice, from A to B between $t_A$ and $t_B$.



# Theory of the Double Layer in Water-in-Salt Electrolytes

*Resulting from a recent collaboration with Michael McEldrew (MIT), Zachary Goodwin presents the development of a unique continuum level theory.*

Recently, there has been tremendous interest in Water-in-Salt Electrolytes (WiSEs): a class of concentrated electrolytes that exhibit greatly enhanced electrochemical stability windows when compared to dilute aqueous electrolytes and impure room temperature ionic liquids. These electrolytes typically comprise of alkali cations with bulky organic anions in an approximately equal weight ratio to the water in which they are dissolved. WiSEs are of great interest

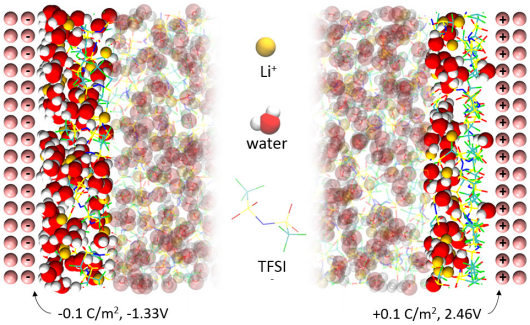
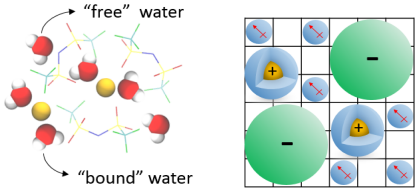



Fig 1 above: MD simulation schematic of 21 m LiTFSI. Fig 2a (below left): Atomistic representation of the LiTFSI fluid structure, detailing the two chemical states of water. Fig 2b (below right): Outline of the continuum 3-component (anion, solvated cation and free water) lattice fluid description.




for use in the next generation of more environmentally friendly lithium-ion batteries, which boast a higher thermal stability compared to existing organic electrolytes.

Previous molecular dynamics (MD) studies illustrated that the enhanced electrochemical stability window could be attributed to the relative depletion of water at positively polarised electrodes. In the presently performed MD simulations, we also found such depletion (Fig 1). It is well accepted that negatively polarised electrodes form a passivating solid-electrolyte interface, which prevents the decomposition of water.

Until the current work, there has been no theoretical description of the electrical double layer of WiSEs, the lack of which is most likely due to the states of ions and water having not been rigorously defined, and because existing equations of states for more than three components of different sizes were extremely cumbersome to use.[1] We developed a methodology to determine the extent of bound and free water in WiSEs, discovering that almost 95% of the water is bound to lithium in its hydration shell, with only 5% of water molecules free to respond to the electrostatic field in the electrical double layer. Furthermore, we generalised a lattice-gas model of asymmetric cations and anions to any number of components (Fig 2b). The continuum model permitted a simple evaluation of the derived modified Poisson-Fermi equation that governs the static electrostatic properties of the electrical double layer. A remarkable agreement was found between the MD simulations and the developed theory (Fig 3). The continuum-level model, which also accounted for ion-ion correlations and dielectric decrement effects, qualitatively captures differences in the electrosorption curves for two WiSEs which vary by the constituent anion. This work was the culmination of a successful collaboration between the groups of Martin Bazant (MIT) and Alexei Kornyshev (ICL).

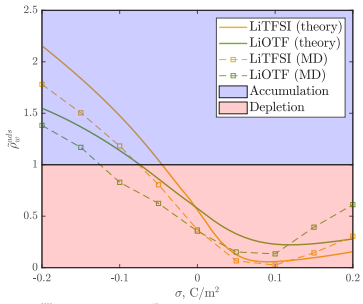



Fig 3: Theoretical and simulated interfacial water sorption isotherms in 21 m LiTFSI and 21 m LiOTF.

1: M.McEldrew, Z. A. H.Goodwin, A. A. Kornyshev, M. Z. Bazant, J Phys Chem Lett, 9, 19, 5840-5846, 2018

# Tuning Electronic Properties via Defect Charge

*Martik Aghajanian shares his current research on using a tight-binding approach to model defects in transition-metal dichalcogenides*

Two-dimensional (2D) electronics is a rapidly growing field with exciting applications in flexible (wearable) technology, and ultrathin microprocessing. Since graphene was first discovered, academics worldwide have continued to express significant interest in the discovery and development of other 2D materials. These include a family of 2D semiconductors named monolayer transition-metal dichalcogenides (ML-TMDs), which have demonstrated spectacular properties that prove useful for channel materials in low-current logic systems.

In realistic conditions, defects dispersed in these materials such as vacancies and charged adsorbates are essential for the performance of junction diodes and photovoltaic devices. Experimental fabrication of adsorbate-engineered samples of TMDs is relatively straightforward. Hence, with the arsenal of materials modelling, a more extensive knowledge of both the electronic and optoelectronic properties of defects in these materials will prove fruitful in the industry of ultrathin device manufacture.

The simulation of charged defects in ML-TMDs comprises several challenging attributes. Firstly, a consequence of the 2D nature of these systems is a weaker dielectric screening than in 3D semiconductors. This corresponds to an electrostatic impurity potential pervading much further away from the defect site. Hence, modelling these systems requires simulating up to $10^4$ atoms in a single monolayer in order to capture the spatial decay of the potential. For first-principles methods like density functional theory (DFT), simulations become progressively more inefficient with an increasing number of atoms. Secondly, acquiring an accurate form of the defect potential is particularly important. For the last 40 years, the interaction between charges (defect-electron, electron-hole) in thin-film semiconductors has been emulated using a model proposed by Leonid Keldysh,[1] which only provides reasonable accuracy at long-range.

For this project, we have implemented a more scalable electronic structure technique, known as tight-binding, to study samples of ML-TMDs over 20 $nm^2$ in area. The screening response, and hence the defect potential, is extracted from a small DFT calculation and easily applied to the tight-binding model. From this simple yet informative multi-scale solution, we obtain defect binding energies, densities (Fig 1), and the prediction of experimental signatures of these defects. Our results for monolayer $MoS_2$, an ML-TMD commonly used in experiments, depict an interesting interplay between the defect potential and the trigonal warping of the electronic structure, giving rise to three-fold symmetric impurity states (Fig 1) which derive from the 2D hydrogen model. In our most recent publication[2] we determine accurate power-law relations between the binding energies of the defect states and the impurity charge, thus, providing a simple model for the prediction of the defect energy structure in monolayer $MoS_2$.

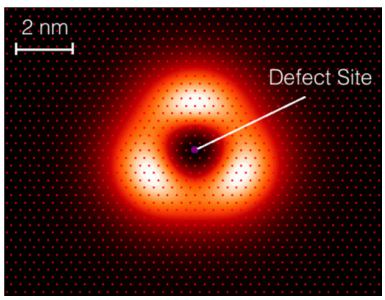



Fig 1: Contribution of a trigonal defect state to the electronic density in Molybdenum disulfide.

1: L. V. Keldysh, Journal of Experimental and Theoretical Physics Letters 29, 658, 1979

2: M. Aghajanian, A. A. Mostofi and J. Lischner, Nature, Scientific Reports 8, 13611, 2018

# Shining a Light on Topological Nanophotonics

*New destinations: Marie Rider outlines the journey from topological insulators to topological nanophotonics*

Imagine that you're set down on an unknown surface, and all you know is that you're standing on either a sphere or a torus. You have limited tools with you and so can only make local measurements on the geometry of the surface where you're standing. How do you tell which type of surface you're on? It turns out that you're going to struggle. A local measurement of the surface where you're standing won't tell you about its topology (global properties). To tell for certain if you're standing on a sphere or a torus, you would have to wander the surface making a string of local measurements, thus making a global measurement to see if there's a hole in the system or not.

Topology can also arise in condensed matter systems, when the Hilbert space describing the electrons of a material has a non-trivial topology. This forces us away from the idea of local order parameters (such as mass density and magnetization), and instead the phase of the material will be described by a topological order parameter (akin to how many holes a sphere or a torus has). Topological insulators (TIs) are one example of such systems. Unlike topologically trivial insulators, the topology manifested in the band-structure of the insulator results in the addition of topological conducting surface states, which are robust against perturbation. Much like how perturbing the surface of a sphere without puncturing it won't result in a torus, perturbing the Hamiltonian of the TI won't remove the conducting states. This remarkable robustness of the surface states makes them of interest in quantum optics and quantum information.

Going further, research is in full swing to understand how these materials interact with light and if they can be reproduced in purely photonic systems. Can we make topological protected photonic states? With a resolute yes we enter the thriving realm of topological photonics. By irradiating TIs with light, the photons interact with both the topological surface states and the insulating bulk, resulting in topologically modified photons. Topological photonic systems can also be produced with no TI in sight. The introduction of light into a system with periodic permittivity reproduces the Hamiltonian of a topological electronic system and the topologically protected states that come with it. However, for purely photonic systems, we work with bosonic rather than fermionic states, so the implementation of topology in these systems requires new paradigms.

Shrinking these systems to the nanoscale, the enhanced sensitivity of nanoscale structures can be combined with the protection of topological photonic states, allowing for the precise control of photons at the nanoscale. In our research group, we study topological nanostructures interacting with light (Fig 1), and photonic platforms which support visible or near-IR topological photonic states. These systems are a step towards addressing the THz gap (the frequency range for which almost no feasible sources or detectors exist), with the potential for topological quantum dots and THz lasers, and deep subwavelength microscopy. The field of topological nanophotonics provides many exciting theoretical and experimental challenges with much to be accomplished.[1]

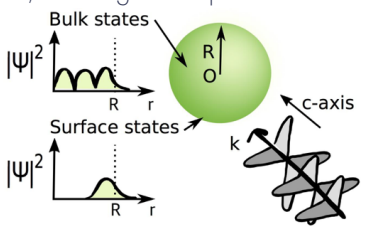
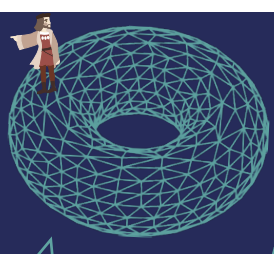



Fig 1: TI nanoparticle interacting with light

1: M. Rider, S. J. Palmer, S. R. Pocock, X. Xiao, P. A. Huidobro and V. Giannini, J. Appl. Phys., 125, 000000 (2019), doi: 10.1063/1.5086433

Exploring different topologies

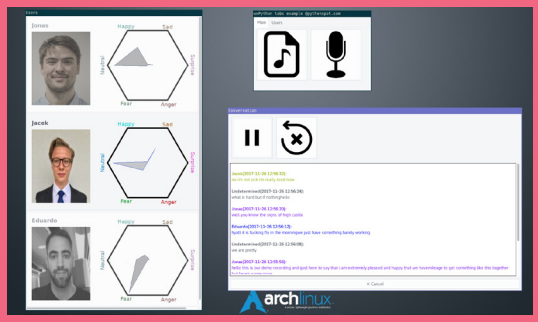


# CDT Life

Catch up on what the CDT has been up to in the last 12 months

## Ready, Set, Hack!

*Jonas Verschueren recounts a 24 hour coding whirlwind when attending Oxford Hack with fellow members of cohort 6: Eduardo Ramos-Fernandez and Jacek Golebiowski*



The speemo interface evaluating the emotional value of different speech (credit: J. Verschueren)

At the crack of dawn on Saturday the 25th of November 2017, Jacek, Edu and I were waiting just outside Victoria Coach Station for the 7.25am Oxford Tube. Why would anyone do that to themselves? Well, we couldn't think of a better way to spend our weekend than going to OxfordHack 2017, a Major League Hacking event organised at the University of Oxford.

The main part of these so-called hackathons is a 24 hour non-stop coding session in which teams produce a little - mainly a proof of concept - software or hardware related project. These then get assessed by a panel of judges who assign winners in different categories. As you can imagine, these events are well supported by big companies who treat it as a big HR event.

We decided to code a little app that would assess the emotional value of some spoken text. To do this we tied together 3 bits. Firstly, given access to a speech-to-text Microsoft API, we utilised it to perform voice recognition and translate spoken words to written text. The outputted text was then

## Experiencing the Experimental

*A trip to BP's headquarters gave cohort 9 the opportunity to see how theory and simulation complements experiment, Matthew Okenyi and Carles Rafols i Belles share the experience.*

On 24 May 2018, we in cohort 9 took a break from our respective projects and gathered together for a visit to BP's facility at Pangbourne. The global headquarters of BP's lubricant business, Pangbourne is one of the main technology centres and the site of formulation and experimental testing of the many products under BP's Castrol brand. Computational modelling is playing an increasingly important role in the development of these high-value products, and so the visit was a good opportunity to observe the tangible impact of work similar to that being carried out in the CDT.

The day started with a tour of the experimental labs, where precise measurements of the viscosity of newly formulated oils are made. It was interesting to experience first-hand an example of how the theoretical prediction of a physical quantity like a liquid's viscosity is ultimately validated. The variety of BP's onsite testing capability was impressive. As well as viscosity measurements, the performance of engines for cars, trucks and motorcycles are also investigated using automated test rigs in order to achieve accurately repeatable experimental conditions.

Following the tour, we split into two groups, and were each presented with a different modelling problem proposed by two CDT PhD students working on different BP projects. The first problem was put forward by Eduardo Ramos Fernández (cohort 6) and involved the multiscale modelling of wear and friction between a lubricant and a solid surface. Understanding how lubricants interact with a surface is crucial for the development of tailored high-efficiency lubricants but different effects take place at different scales and a unified modelling is still lacking.

The second problem came from Carles Rafols i Belles of our cohort and concerned sweet corrosion of carbon and low alloy steel (CLAS). It is crucial to understand this phenomenon in order to extend the lifetimes of offshore and onshore oil and gas pipelines and related oil field equipment. However, the mechanism of the nucleation of siderite ($FeCO_3$) scales on CLAS is poorly understood.

fed into a neural network that we trained on a bunch of tweets, labelled with their emotional value. Finally, we tied all of the processes together in a user interface that displayed the results clearly. The code for all this is publicly available and can be inspected (at your own risk!) and contributed to at https://github.com/TSM-Hackers/speemo

After a sleepless night fuelled by snacks, pizza, sugary drinks and the pure excitement of coding, it was time for the judges to come and have a look at what we'd produced. We were delighted when they selected our project for the final so we could present it to all of the 350 attendees. Never have I given a less prepared presentation, having to give a live demonstration of our inevitably buggy app combined with not having slept in a very long time. But it went surprisingly ok.

All in all, we really enjoyed it. We definitely encourage anyone interested in putting a proof of concept project together quickly and amassing some free T-shirts in the process to go to a hackathon event. Besides, taking time off over the weekend is overrated anyway.

After fruitful discussions, we agreed that a possible approach to tackle the first problem would be to combine modelling techniques that operated at different scales, such as Molecular Dynamics and Phase Field. For the second problem, we decided that using Monte Carlo simulations was a good initial step to understand the early stages of sweet corrosion.

We were grateful for the chance to see the inner workings of an organization that employs theory, simulation and experimental approaches. Such opportunities are rare for most of us in the cohort (although many of us were eager to escape that messy world of test tubes and Bunsen burners during our PhDs!). We would like to thank our cohort mentor, Prof. Daniele Dini, and Eduardo, who accompanied us on the trip, and all of the members of staff at Pangbourne for their stimulating insights.

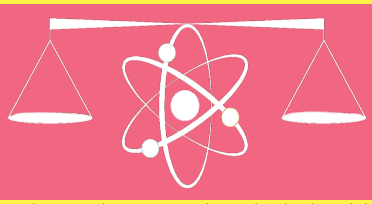
# Taking on Science and Ethics

*Gabriele Coiana reports on organising a successful CDT Festival of Science & Engineering*

As this year's representative for the TSM-CDT, I greatly enjoyed experiencing being a member of the organising committee for the CDT Festival of Science & Engineering. The festival is run every year as a collaboration between all of the CDTs at Imperial, and every year it has a different topic. The theme always involves science – of course – but in a relationship with other fields. This year we decided on a particularly challenging theme: "Science and Ethics". We thought that ethical questions are increasingly important nowadays, especially since the progress of technology impacts the human sphere in a variety of ways, and science is increasingly required to show an awareness of this. We invited experts, researchers and professors to give talks across a range of fields: sustainable innovation, climate change, moral philosophy & artificial intelligence, genome editing and quantum technologies. The talks focussed on how their research relates to Ethics; what more they think should be done in this direction, and how they think the world will progress and change.

Left: One of the engaging talks during the CDT Festival of Science which took on a stimulating Science and Ethics theme (right)

(Credit: G. Coiana)



Moreover, to differentiate the activities we decided to introduce interactive elements. The audience could make comments about the whole range of topics (directly from their smartphones), answer questions, vote, and... Pandemic! Pandemic is a virtual story in which the spectators are asked to say how they would behave in the situation reproduced by the film projected on the screen. Based on how the majority votes, the story continues in a different way. A unique experience, Pandemic makes you reflect on how ethical questions define your whole life.

From my perspective, the Science and Ethics topic was both extremely interesting and challenging. The willingness and effort that the organising team – comprised of 11 CDTs – showed in creating such an engaging and enjoyable event were really worth it!

# Authentity

*Sophie Finnigan recounts a May break away from research*

Members of cohort 8 headed to Cumberland Lodge for the 2018 edition of Piero Vitelli's ingenious Authentity. The personal development course unites the TSM-CDT with CDTs from Bristol, Sheffield and Manchester, resulting in a complementary social experience and an opportunity to meet other PhD researchers. Packing a plethora of group exercises and activities across two and a half days, the course is unique in its construction and delivery. The main and culminating task of the course was for groups to create and pitch an activity-based workshop for children that taught them about an aspect of failure. The aim of the course isn't some grand transformative process but that everyone leaves with either a change in perspective or a little more personal insight than what they arrived with. This was certainly true for me!

An interesting theme raised over the experience was the secret to constructing a successful team. I had always believed that a team needs a cocktail of personalities, who will naturally adopt different roles, in order to work. During Authentity though, I found myself in a team of very similar people. Initially, my preconception made me a bit apprehensive about how well we were going to work over the next couple of days. The actual experience, however, was surprising. While we were perhaps all a little too quiet and reflective sometimes, we actually worked effectively and successfully together and all had a laugh in the process! The result was one of the best team experiences I have ever had and an enjoyable few days. So what had made us work so well? Piero shared with us an eye-opening study run by Google that researched what exactly makes a good team tick. The result? They couldn't find one, there was no secret formula, which can be quite disconcerting for a scientist! Instead, the idea of 'psychological safety' was raised. Psychological safety is the idea of feeling comfortable enough to be yourself and to share your thoughts within a team. The concept seems so obvious once pointed out and was the apparent key to our team's success during Authentity. However, it wasn't something that I had been conscious of previously. The idea of trying to introduce psychological safety within any future team environment was one of many enlightening experiences for me from the course. Authentity was more than just your average 'soft skills' course and I think that everyone did leave at least a little more self-aware.

# TSM Annual Conference

June saw another successful Annual Conference and an opportunity for the CDT students to showcase their research.

Cohort 6 saw out their final TSM conference by presenting short talks on their research. A high standard meant that the prize for best talk was well fought for, with the eventual win split between Chris Ablitt ('Ruddlesden-Popper and the Mystery of the Shrinking Ceramic') and Jonas Verschueren ('The role of dislocation-lattice interactions in the mobility of dislocations in the pure-glide regime').

Engaging key notes were given by MIT Professor Craig Carter and TSM Alumnus Ben Kaube (cohort 3), who gave an insight into succeeding in the start-up world.

Above: Authentity was packed with full group and team activities; one of the teams who successfully took on failure.

Below: Craig Carter holds a captivated CDT audience and the TSM Annual Conference prize winners.

Left: Cohort 8 pre- and post- Authentity: gaining Syed and some personal insight (credit S. Finnigan). Right: The master at work as Adrian gives a talk at Hermes 2018 (credit: Hermes Comms).

# A Fond Farewell

## TYC Student Day

The Annual TYC Student Day, hosted this year by UCL, displayed the diverse research encompassed by the Centre.

The TSM-CDT was well represented, with Lars Blumenthal, Jacek Golebiowski, Iacopo Rovelli and Hikmatyar Hasan (all cohort 6) all invited to present their research in short talks. Success in the high calibre poster competition saw Sophie Finnigan (cohort 8) jointly awarded the best poster prize for her poster titled "Modelling the Environmental Decomposition of the Nerve Agent VX".

After an enlightening keynote by Prof Sally Price, Dr Andrea Taroni closed an excellent day with a unique insight into the world of being Chief Editor at Nature.

Posters galore at the TSM-CDT Annual Conference.

*Following his retirement from an impressive career, of which the TSM-CDT is just one part, Arash Mostofi acknowledges the achievments of Adrian Sutton.*


Professor Adrian Sutton FRS formally retired from Imperial College in 2018. Adrian joined Imperial in 2005 as Professor of Nanotechnology and Head of the Condensed Matter Theory group in the Department of Physics. He soon set about his long-standing dream to create a centre for education and research in theoretical materials physics, which in 2009 resulted in the creation of the Centre for Doctoral Training in Theory and Simulation of Materials (TSM-CDT), with Adrian as its founding Director. Under his leadership, the TSM-CDT flourished and set the gold-standard for high-quality postgraduate training, his achievement being recognised by the College with the award of the 2012 Rector's Medal for Outstanding Innovation in Teaching. We all wish Adrian a very happy and fruitful retirement!

## Remembering Alessio

*September tragically robbed us of one of both the brightest minds and personalities of the TSM-CDT. Gabriele Coiana remembers Alessio Bevilacqua.*

Alessio Bevilacqua (cohort 9) was an accomplished mechanical engineer and materials scientist. Before joining the CDT, he obtained his MSc at the Politecnico di Torino, in Italy. He also spent time in the US on an academic exchange programme, and to conduct his thesis research at MIT in Boston.

At Imperial, he worked with Dr Stefano Angioletti-Uberti on the interactions between nanoparticles to be used as drugs to combat the influenza virus. He addressed this problem both with simulations and theoretical techniques. Recently, he had derived an analytical formula – to be compared with the numerical simulations – to evaluate the energy of the interactions, which he had hoped to publish soon. He was brilliant.

But this is only one side of Alessio. Here is his legacy: his incredible passion, his friendship, his loyalty, his intelligence, his hilarity, his righteousness, his empathy for anyone and everyone, his "let's go for a beer and forget about problems!", his extreme love for life.

This and much more was Alessio: a real friend and a light that will always shine for those who knew him.

Image credits (Alessio Bevilacqua and posters above): M. Smith

**Luca Reali**
**NuMat, Seattle, USA**

The conference was very focussed on my topic, and a great opportunity for networking. I found Seattle to be a lovely city, perhaps it was the postcard-like weather that we had or that it was the first time for me among that many skyscrapers. The only disappointing thing was the size of the portions at the restaurants, which did not live up to my expectations!

**Martik Aghajanian**
**APS March Meeting, Los Angeles, USA**

As one of the largest Physics conferences in the world, APS March Meeting provided attendees with extensive opportunities, both to delve into their field of study and to learn more about research in other sub-disciplines. LA lived up to its glamourous reputation with captivating skylines, and a diverse array of bars and eateries.

Above: Seattle skyline. Below: The MSE congress stage is set


# From MSc to MSE

**Join cohort 9 on their MSc conference trip and discover Darmstadt, Germany and the MSE Congress**

On a clear Tuesday in late September, twelve members of cohort 9 took a short flight from Heathrow to Frankfurt am Main, to attend the Material Science and Engineering (MSE) Congress 2018. After checking in to our hotel, we wandered the city centre to get a feel for the area. Although the evening was quiet, we could still admire the monument to Louis I, Grand Duke of Hesse, which dominates the central plaza. We ordered dinner from a cheerfully decorated burger restaurant and went to sleep looking forward to the conference ahead of us.

The MSE Congress was hosted by the Technische Universität Darmstadt and was comprised of six broad themes spanning theory, experimentation and problem-driven engineering. One of the Congress's strengths was the variety of research that was presented. Each of our adopted research fields was well represented at the Congress, and we benefited from interacting with researchers at the forefront of fields as diverse as materials characterization; atomistic and continuum-scale modelling; and novel machine learning techniques.

In particular, attending some of the experimental talks enriched our understanding of the context in which our theory and simulation projects are embedded.

On Friday evening, a group of us visited Frankfurt, Darmstadt's metropolitan neighbour and financial centre of the country. We approached the Altstadt by following an authentic marching band, whose old-fashioned music and charm imbued the city with the spirit of the imminently commencing Oktoberfest. Although we had to depart before the Steins began to slosh, we took the opportunity to try Handkäse, another Hessian delicacy – sehr lecker!

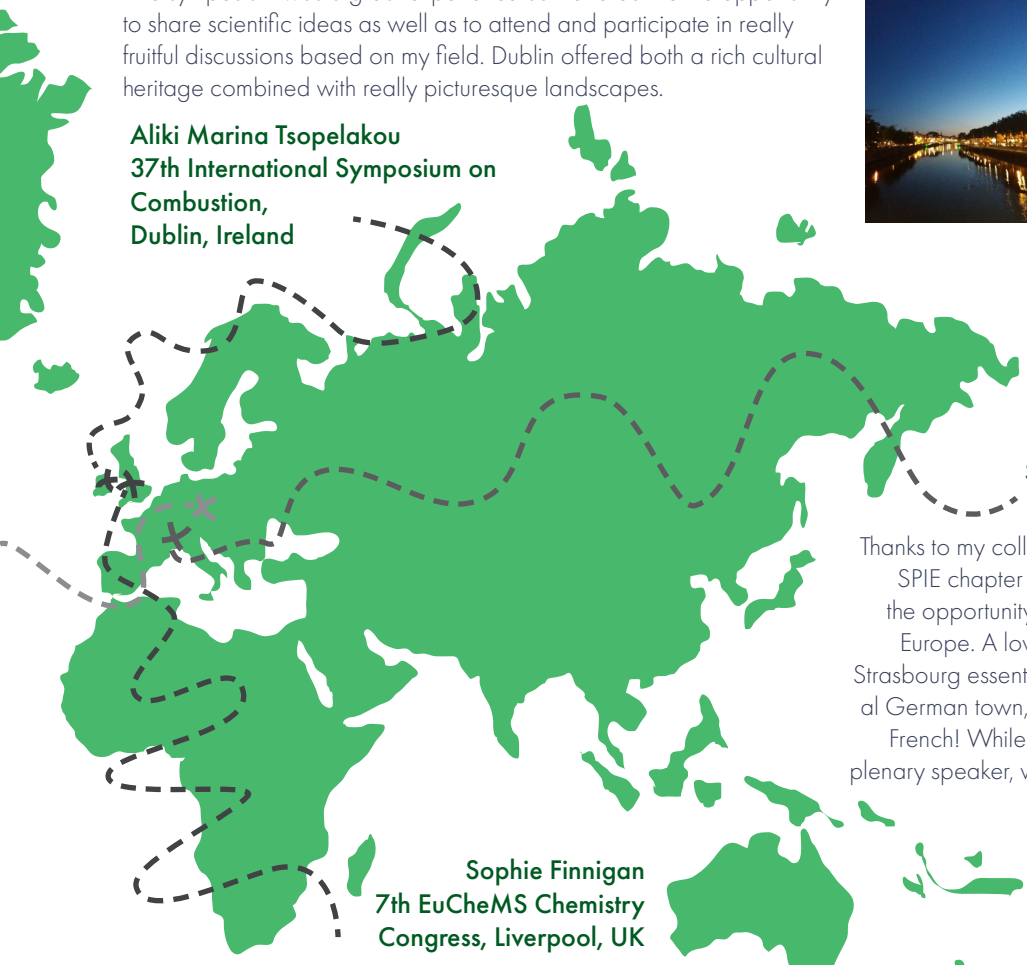
We ended our stay in Darmstadt by visiting the church of St Ludwig, which towers over the central high street. The building's interior was breathtaking; we could only admire the symmetry and beauty of the domed ceiling and Ionic-style columns.

On reflection, the MSE Congress is perfect for anyone interested in the nexus between materials modelling and engineering – both theoreticians and experimentalists alike. Finally, thanks to our cohort mentor, Prof. Daniele Dini, for accompanying us, and to Miranda Smith and Naho Ollason for their organising wizardry.

Image credits: L. Reali and D. Ho

# Jetset, Go!

**Pack your bags and explore a fascinating array of conferences and destinations with members of the CDT**



### Aliki Marina Tsopelakou
### 37th International Symposium on Combustion, Dublin, Ireland

The symposium was a great experience as it offered me the opportunity to share scientific ideas as well as to attend and participate in really fruitful discussions based on my field. Dublin offered both a rich cultural heritage combined with really picturesque landscapes.

Image credits: E. Galiffi and A. M. Tsopelakou

### Emanuele Galiffi
### SPIE Photonics Europe, Strasbourg, France

Thanks to my collaboration with the OSA/SPIE chapter at Imperial, I was offered the opportunity to attend SPIE Photonics Europe. A lovely, historically rich town, Strasbourg essentially looks like a traditional German town, but where people speak French! While there, I had a chat with a plenary speaker, which resulted in a current collaboration.

### Sophie Finnigan
### 7th EuCheMS Chemistry Congress, Liverpool, UK

Offering a broad programme including physical, analytical and theoretical chemistry, the conference provided a varied insight into current research and global challenges. Liverpool was as enjoyable as ever, and it was great to play the tour guide to Masahiro, a Japanese MRes student from my research group. The conference dinner was hosted in the Anglican cathedral, resulting in one of the most memorable dining experiences.

Image credits: S. Finnigan

Top right: Emanuele in Strasbourg and Dublin blue hues. Above: Liverpool Csathedral and the Bootleg Beatles entertaining the EuCheMS crowd. Left: Darmstadt dinners, draughts, the church of St Ludwig and the central plaza.

Image credits: D. Ho

**How did you hear about Hermes and what made you get involved?**

Bianca (BP): I found out about Hermes 2016 from the Psi-k mailing list and thought it sounded interesting. It was unlike any conference I had been to. I absolutely loved broadening my horizons by learning about other computational methods used in materials modelling. The science communication workshops were genuinely helpful and fun, and sharing accommodation and meals on site with participants and speakers meant getting to know fellow researchers in a much more relaxed way. Nikoletta and I were actually roommates at Hermes 2016 and we got along incredibly well, so we were excited to work together to deliver the Hermes experience to a new cohort of students in 2018!

Patrick (PR): My supervisor told me about it!

Nikoletta (NP): I heard about it through our CDT and my incredible experience attending in 2016 inspired me to help organise the next version in 2018 and offer students the opportunity to experience what I had.

**As the most diverse team yet to organise Hermes, what do you think this brought to the event?**

BP: I truly believe having a diverse team can only be a good thing. In terms of organising Hermes 2018, it meant we had access to a huge network through our committee, as well as a range of opinions, skills and represented disciplines which, I suspect, resulted in a more well-rounded summer school.

Fangyuan (FG): Different people provided different opinions, enabling us to have a broader, more global perspective.

**What was the biggest organising challenge?**

Roya (RM): Resolving some of the conflicts of interest between organisers.

BP: In my opinion it is both a strength and weakness to have an organising committee spread around the world, but certainly one of the biggest challenges we faced was arranging video conference meeting dates and times which would work for everyone. What with the different time zones and a big committee with busy schedules, it bordered on impossible for everyone to be able to attend most meetings. I think it's also safe to say that balancing the conference organising on top of a PhD was a challenge and learning experience for all the organisers.

PR: Yeah, definitely managing the time spent on Hermes with the time spent on research

> "...our team had pulled off what seemed to be a valuable event..."

**What was your highlight of the conference?**

NP: The multi-national character of the summer school with students attending from many different countries.

PR: Actually meeting all of the students who had come from all across the EU and further afield.

FG: I think one of the highlights was the science communication challenge which involved giving a short 3-minutes presentation summarising your PhD without any visual aids. Following our science communication workshops, this was a great opportunity to put into practice the skills learned, with prizes presented to those who demonstrated the best science communication skills.

BP: Seeing everything we had worked hard on for nearly two years come together at Hermes 2018 was incredibly rewarding. I received positive feedback from several participants, including one who said that Hermes was "life-changing" for them. That really makes all the energy we put into this conference feel worthwhile!

**Describe your Hermes experience in 3 words.**

PR: Enjoyable, proud, tiring!

# Inside Hermes

## Hermes Summer School uniquely hosts Materials Modelling Masterclasses and Science Communication experts. Experience the inside track from the 2018 organising team

Image credit: Hermes Comms

## Meet some of the organsing team:

### Fangyuan Gu

**Hermes Role:** Communications: event advertisement, attendees and speaker communication

**Research:** TSM-CDT PhD. Utilising ultrafast optical excitations to control structural changes in multiferroic materials.

### Nikoletta Prastiti

**Hermes Role:** Co-President

**Research:** TSM-CDT PhD. Modelling fatigue at the microscale for important alloys used in the aerospace industry.

### Bianca Provost

**Hermes Role:** Co-President

**Research:** Surface Science PhD (University of Cambridge). Understanding the mode of action of molecules used to protect steel surfaces from acid corrosion through atomistic modelling.

### Roya Moghaddasi

**Hermes Role:** Selecting and inviting speakers

**Research:** Research Assistant (University of Toronto). Using numerical schemes to understand the role of quantum effects in the thermal conduction properties of interacting systems.

### Patrick Rowe

**Hermes Role:** Event funding and sponsorship

**Research:** Computational Physics PhD (UCL). Developing interatomic potentials by machine learning.

RM: Productive, multidisciplinary, amazing location (slightly cheating!)

FG: pleasant, shared, communicative.

NP: Enlightening, thrilling, exciting.

BP: Unforgettable, enriching, important.

**How did it feel when the conference came to a close?**

PR: A little bit strange! We'd been working on organising the conference for close to two years, and it had become quite a large part of our routine, especially in the weeks actually leading up to the event. When it was over, there was a sense of relief that the event had been such a success, but I was also a bit melancholic that it was finished.

NP: A mix of happiness, satisfaction and relief that we had delivered another successful version of the summer school.

BP: I also had quite mixed emotions. I felt some relief because prior to and during the conference, we had many responsibilities to ensure the school ran smoothly. A particular stress was ensuring that everything ran according to schedule so that no one would miss lunch or dinner! Aside from relief, I also felt some sadness that the school was over, that we would no longer meet as a committee and that we had to leave the beautiful Cumberland Lodge. Mainly though, I felt an incredible sense of accomplishment

and joy: our team had pulled off what seemed to be a valuable event for our students and speakers, and I was lucky enough to network with wonderful researchers and learn new things.

**What would be your one piece of advice to the next organising committee?**

BP: Start early! Most things took us longer than expected, and even when they didn't, it was better for everyone when things had been started in advance.

PR: If you spread the work out it's so much easier.

NP: Keep track of time.

FG: Enjoy yourselves and try new ideas.

RM: Work well as a team and solve any conflicts from the beginning.

**Forget dinner party guests, who would be your dream speaker to book for a conference?**

PR: Richard Feynman is widely renowned for being one of the greatest scientific communicators of modern history, so probably him.

BP: Professor Emily Carter (Princeton).

FG: Prof. Nicola Spaldin (ETH, Zurich).

Prize winners, presentations and workshops all within the beautiful Windsor park.

Image credits top to bottom: A. Mostofi, Hermes Comms, J. Smutna

## ...and From the Outside? Jana Smutna shares an attendee account

I had the pleasure to attend Hermes along with a host of postgraduate students from both the CDT and across the globe. Hermes focusses on materials modelling and science communication. The materials modelling workshops themselves spanned length scales from electronic structure methods up to macro-scale modelling. The four days were packed with talks, workshops and opportunities to practice the newly learned skills, from using finite element modelling to a 3 minute thesis competition.

The thing that makes Hermes really special is that it's organised by PhD students for PhD students, and no matter what you're currently studying or want to do in the future, there is something new to learn. Even though I had a pretty good idea about density functional theory (DFT) through my own research (in fact, some of my own talks include a brief overview of the method) the introductory talk on how DFT works for a complete beginner was definitely the best explanation I have seen, and helped me to understand a bit more how it all fits together. In fact, the quality of talks was outstanding, and I think I learned as much about science communication from the science talks as I did from the ones about how to be a good communicator.

There was also plenty of time and opportunity to interact with fellow students and speakers. On the more formal side, a couple of Q&A panels had been organised, mainly focusing on careers post PhD, in and outside of academia, science and non-science based roles. It really opened my eyes to the spectrum of opportunities available and important things to consider when applying for a job. Most of the speakers were also available for a drink at the Cumberland Lodge bar in the evening, giving out tips and sharing experiences.

When it comes to meeting fellow students, there was a poster session, lots of group discussion and presentation activities, and of course the aforementioned bar. Some of these connections will last long after leaving Cumberland Lodge. In fact, some of the participants will be organising Hermes 2020, and while I didn't sign up for this particular task, it was still great to see the present and future organisers in London recently.

Hermes is hard to summarise, since it offers such a variety of activities. It is a wonder that it was possible to pack so much into just four days, and four days I will remember fondly for a long time!

# Code for Creation

Each year, the Royal Society holds its largest outreach event: the Royal Society Summer Science Exhibition (RSSSE), celebrating the cutting edge of UK science research.

The exhibit selection process is highly competitive with 21 spaces up for grabs. Not ones to shy away from a challenge, Arash Mostofi, Johannes Lischner and Simon Foster crafted a proposal to showcase the research and ethos of the CDT. The stand aimed to communicate how computational advances are unlocking the potential of theory and simulation as key tools in bridging length scales to understand, design and discover materials.

Selling the ground-breaking nature of our research, the proposal passed the selection process and success! Code for Creation was born.

Now the real challenge stood ahead: to design, build and fill an exhibition stand which engaged volunteers and displayed our research. Let alone finding the volunteering workforce needed to deliver it all during the week of the exhibition itself...

Step forward Emanuele Galiffi (cohort 8) and a host of TSM-CDT students. Experience the journey, from concept to event, of Code for Creation.

## January: 6 months to go

An unusual silence fell in Room 113, Whiteley, as Johannes asked who would be up for leading the preparation of the 2018 RSSSE TSM stand. The mountain of a role involved managing a £20K budget to bring a concept, and a name which ~10 people had just spent 2 hours trying to choose, to reality. The long stillness was eventually broken by a tentative hand raise. Somehow thrilled by the idea of challenging himself on a leadership role that he felt was way above his level of confidence, not to mention experience, Emanuele stepped up to the role.

The venture of designing and delivering a successful exhibition stand was not one to be underestimated. The numerous tasks included: managing finances, designing the stand itself, populating said stand with diverse, interactive activities, producing a promotional video, launching social media accounts, creating handouts... The list seemed endless and more manpower was going to be needed. A pizza-driven hackathon did not fulfil its original purpose of attracting more volunteers, but it did help bond those already interested. A tight team of well-motivated volunteers began to establish, which would prove crucial later on.

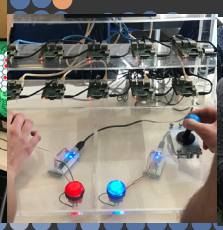
While ideas were plenty, the conception of activities which were both fun and engaging but also effective at communicating our research was tough. The first couple of months were spent evolving, discussing and refining ideas into proposals. A second challenge was maintaining a cohesive message across the stand while also inventing activities which showcased different aspects of our research. In the end, a neat strap-line: 'Understand, Design and Discover' was conceived that encompassed the exhibit concept.

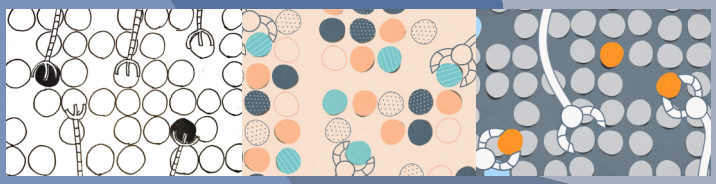
From the impressive programming skills of our core group of volunteers, the selected activity proposals began to develop under this strapline. For 'Understand' we had "Nuclear Bake Off", a late turnaround after an initial idea of visualising stresses and strains forming from user interaction was shelved months into the process. 'Design' was covered by "Defect Drop" and the 'Discover' element arose from a collaboration with Aron Walsh's Materials Design group to develop a "Materials Discovery App". However, plagued by development difficulties, the app remained little more than a promising idea over the following few months. The final activity showcased the power of modern supercomputers with a multiplayer game against a Raspberry-Pi cluster.

Meanwhile, as the activities developed, work was ongoing to create the promotional video and a Code for Creation 'brand'. Thomas, the Tier 2 HPC system hosted by the Materials and Molecular Modelling Hub that is led by the Thomas Young Centre, was


introduced as a character and a logo. An animation company, TinMouse, were brought on board and transformed both Thomas and an initial sketched out storyboard to life. However, achieving a balance between maintaining scientific accuracy and delivering the story of our stand in an accessible manner for the general public was a difficult process. There were many, surprisingly intense, discussions on just how to visualise atoms and defect formation in a fun but accurate way... Aiming the scientific level of the exhibit to the right audience was a prevalent challenge across all aspects of the stand. The expected diversity of the RSSSE crowd meant that we had to communicate our research to an audience who might not have studied science for a very long time! Fortunately, we had Simon Foster, the Physics department and CDT Outreach Officer, to guide us through.

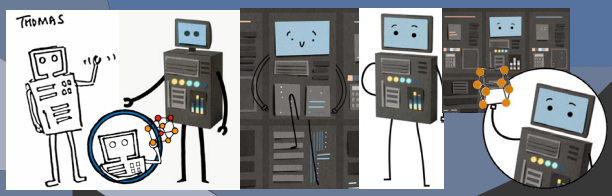
Below: Activity development and even our volunteers couldn't resist testing at the Imperial Festival. Above: Banners, T-shirts and tattoos (elegantly modelled by Johannes).





# How do you bring a supercomputer to life?

The friendly face of Code for Creation and a brilliant video evolved from initial sketches by Sophie Finnigan




### Imperial Festival: 2 months to go

Every year, Imperial hold their own outreach festival which showcases the impressive host of university research for families and alumni. The weekend-long event was the perfect testing ground, with Defect Drop and the Raspberry-Pi Arcade making successful debuts. The experience highlighted improvements to be made and showed the level of durability that the activities (and volunteers!) were going to require to see out a full week. With us all officially on count-down mode to the event though, there had so far been no sighting of the Materials Design app and at this point, Nuclear Bake Off had barely begun cooking.

### End of May: 1 month to go

As the event drew near, the exhibit began to become more tangible. The deadline for the final video was successfully met and Code for Creation hit Twitter to start building excitement. The last month was filled with a hurricane of preparation as a website, 3D prints and other handouts, T-shirts, and the stand itself all began to materialise. Somehow, Emanuele managed to keep track of it all and calmly lead us through with, miraculously, nothing forgotten.

### 22nd June: 1 week to go

The Friday before the event finally saw all four activities present in one room! The bulk of the volunteering team assembled for some final training and to experience what they would be experts on in just a week's time. The excitement started to build as we got the chance to trial the activities and to share what we had all been busy developing. The Materials Discovery App made its exciting first appearance, although the initial prototype ultimately saw a lot of last-minute development! The delivery of the stand pieces and banners in the week gave us a chance to give the building and dismantling a dry run (a jigsaw experience to match no other!) and we knew that the next time we'd see the stand it would be for the real thing.

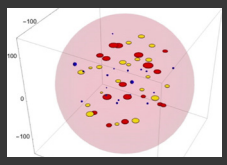
### 30th June: 2 days to go

Finally, it was time. Banners, boxes, monitors, the stand and wires galore were all loaded into the back of the Imperial Physics van for the short (and early!) morning drive to the Royal Society. To greet us on the floor was a taped out area of carpet, overlooked by Sir Isaac Newton himself, just waiting to be transformed. The practice build came in handy as the exhibit was constructed and finishing touches were put to the Raspberry-Pi custom built arcade. With a final last minute upgrade to the app version, even the 'Materials Design App' was raring to go. We were ready!


Project build it: Setting up the RSSSE exhibit.

Image credits: S. Finnigan, S. Foster and E. Galiffi

Developer: Iacopo Rovelli



An interactive 3D simulator of defect annealing for fusion reactors, Nuclear Bake Off opens with an introductory simulation of a collision cascade causing radiation damage in the reactor walls.

The player then selects their 'baking' conditions: setting the defect distribution and temperature. The aim is to achieve the quickest annealing time and to understand the underlying healing processes occurring.

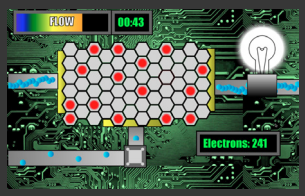
How Heating Helps Healing

# Nuclear Bake Off

# Defect Drop

## Designing Devices by Defects

Boasting a retro game controller, vivid graphics and some purpose-built electronic music from Tomos, Defect Drop was a hit with all ages!




Faced with a poorly performing transistor, the player has to optimise the graphene by doping it with adsorbate atoms. The arrangement of the defects on the graphene has to be designed to maximise the electron flow, illustrating both materials design through simulation and the potential of 2D-materials for electronic devices.

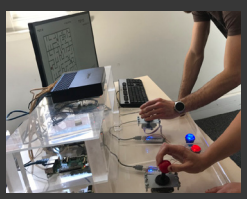
Developers: Martik Aghajanian & Tomos Wells

# Discover the Stand!

# Raspberry-Pi Arcade

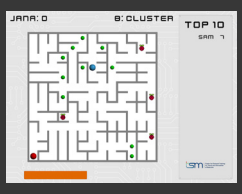
## Pitting you against the power of parallelisation!

Ingeniously programmed and housed in a custom-built arcade, the Raspberry-Pi arcade is a cooperative maze game.



The two players negotiate a maze, collecting points before the Pis. As the players progress through the levels, the number of Raspberry-Pis they are competing against increases. The Pis work in parallel, moving around the maze by random walks and making the task of beating the growing cluster (and knocking Arash off the leaderboard) become devilishly hard!

Developers: Sam Palmer, Jana Smutna, Charles Penny and Ignacio Bordeu Weldt

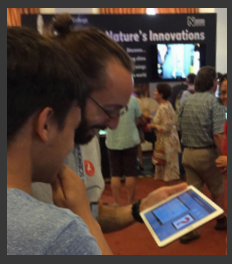



# Materials Discovery Challenge

## Predicting Perovskites

The Materials Discovery App introduces the power of computers in material screening as visitors search for viable perovskite structures.

The neutral combinations of two user-selected metals and a non-metal are calculated. A successful perovskite crystal is formed if the chosen elements can achieve a stable arrangement in a 1:1:3 ratio. For triumphant users, properties of the perovskite e.g. solar efficiency and cost are then calculated to see if candidates for next-generation solar panels have been discovered.




Developer: Jacob Wilson

Image credits: S. Finnigan

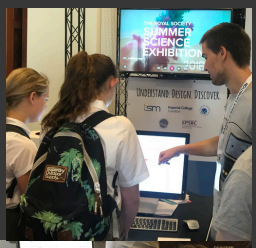

Dressing to impress: volunteers ready for the evening soirées

### Monday 2nd July: Showtime!

In the week where the UK World Cup fever peaked (was football coming home?), the grand doors of the Royal Society finally swung open to the general public. A flood of visitors, from organised school trips to a chaos of families and individuals, kept flowing throughout the full week of the festival. The variety of the audience was astonishing, and two evening soirées even saw some of our lucky volunteers scrub up and deliver our stand to a black-tie crowd of invited guests. The volunteering sessions were intense, but witnessing young and old competing to get on the activity leaderboards, avidly collecting the handouts and walking around with Thomas stickers on made all of the hours spent designing, developing and programming worthwhile. The main reward was interacting with genuinely interested members of the general public who walked away having learnt something new. We also managed to learn some science ourselves by exploring the surrounding, captivating exhibits and hearing about the journeys behind their stands. The scope of topics varied from the complex mysteries of our gut biome to utilising neutrinos to understand the Universe, and it was great for our research to be among them.

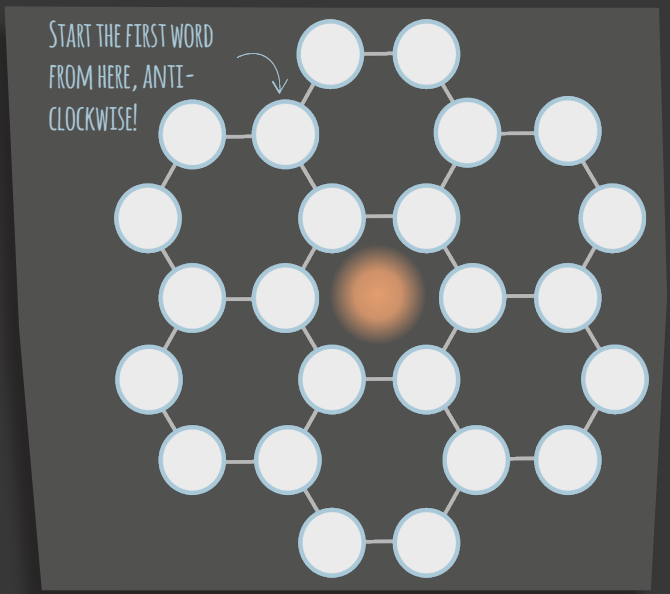
No sooner than it felt like the doors had opened did they close again for the final time. The hubbub of the general public and volunteers was quickly replaced with a flurry of dismantling. Soon, a sea of half-packed boxes, trailing wires, silent screens, and an area of carpet partially marked out with some remaining masking tape, were the only reminders of our exhibit. Overall, everything had come together to deliver a long, hot, but immensely rewarding week. While the journey of the RSSE was over, the legacy of what we had created will continue. The activities will be featuring at the Imperial Lates, the Imperial Festival and hopefully, wider outreach events in the future. Alongside this, everyone involved had gained skills and an experience which will never be forgotten. Without the huge spectrum of unique skills of everyone involved, and Emanuele's impressive leadership, "Code for Creation" would only be little more than a (suspiciously religious-sounding!) name.

By S. Finnigan and E. Glaiffi



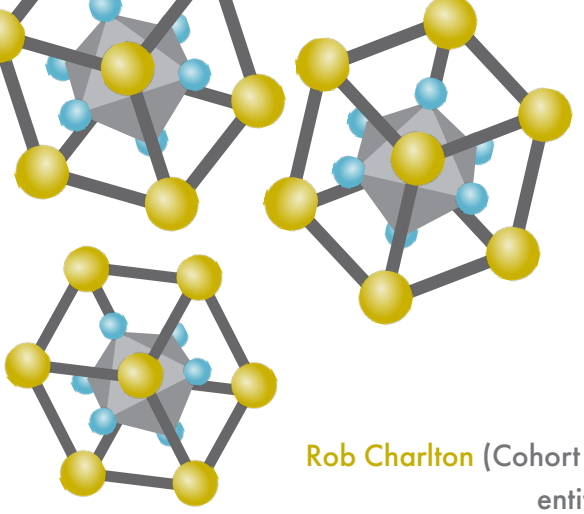


The stand in action with engaged visitors and, below, the joy of topping the leaderboard! (credit: S. Finnigan)




Have a go at one of our handout puzzles! Fill the graphene grid with the 6-letter answers (clockwise or anti-clockwise) to the questions below.

1. OUR SUPERCOMPUTER
2. THE SMALLEST LENGTH SCALE
3. MATERIALS WHICH ARE TYPICALLY GOOD CONDUCTORS
4. _AT_RI_L S_I_N_E
5. MICRO AND MACRO ARE LENGTH _ _ _ _ _ _
6. METER, INCH, FOOT ...?



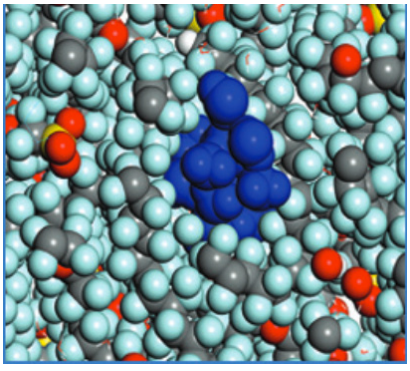
Branching Out: Hear three diverse internship experiences

# Crossing Over to the Commercial Side

**Rob Charlton (Cohort 6) gains perspective of the commerical side of scientific software engineering during his time at BIOVIA**

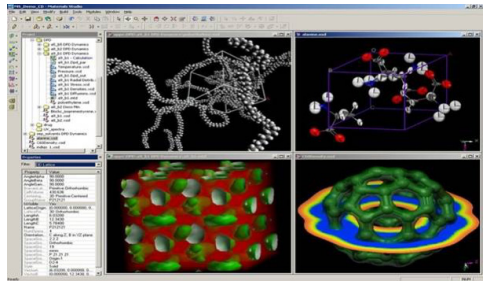
One unique aspect of the TSM-CDT compared to other PhD programmes is the emphasis put on career opportunities outside of academia. With this in mind, during my second year I started looking around at possible internships that could help me gain a feel for work in industry. Then a unique opportunity presented itself at Dassault Systèmes BIOVIA in Cambridge, by virtue of my research using the linear-scaling ONETEP programme.

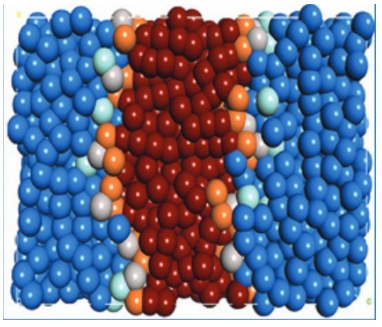
ONETEP is a linear-scaling DFT code written by academics at universities across the UK, commercially available via BIOVIA's Materials Studio software package. Of course, people who work in academic and commercial settings often have different outlooks when it comes to scientific software development. The company were thus keen to have someone with knowledge of the ins and outs of the code come to work with them, to improve the use and integration of ONETEP for the end user. Thus began my three-month placement in Cambridge.



The most striking aspect of the work was how different the outlook was compared to academia. During my PhD research, the majority of the tasks and deadlines were set by myself alone, with occasional discussions with supervisors and collaborators to set forth the overall direction of the PhD. The ability to work by oneself is, of course, an essential and valuable part of PhD work, as you grow to be an independent researcher. By contrast, in a company, there is a far greater emphasis on short-term goals that clearly build towards long-term development.

Even though the work was in a field related to my PhD, I learned an enormous amount during my placement. I was introduced to the world of agile programming, code reviews and build management. All of which enabled me to hone my software development skills with the help of a team of highly experienced scientific software developers. No longer could I hide away in a corner while I focused on a problem facing me during my research. Instead, cooperation within a team was an essential part of the work, with frequent discussions and progress reviews.





Top right: Materials Studio screenshot.
Above: BIOVIA simulation shots

My time at BIOVIA provided an invaluable insight into life beyond university, giving me a far better idea of where my future career prospects may lie. Overall internships are a great opportunity for any PhD student and I'd highly recommend everyone to give it a go.

# Inside the Start Up Machine

## Find out about the inner workings of AI start up Cytora from Alise Virbule (Cohort 6)

After two years of working on my PhD, I took a six month break to try out something completely different: I worked as a data analyst at an AI startup in London's Silicon Roundabout.

This opportunity arose following the careers course organised by the CDT in March 2017. Around this time I had started questioning whether academia was the route that I wanted to stay on, so when I heard that Cytora, an AI startup co-founded by TSM alumnus Dr Aeneas Wiener (cohort 1), was looking for interns, I did not hesitate to apply. My main motivation going into the internship was discovering what the data science craze was all about and to gain some practical skills that would come in handy outside of academia.

As it turned out, one of the most significant learning points was better understanding my work ethic and daily motivation levels, as well as finding out what drives me to do my best at work. During the second year of my PhD I had already started struggling with keeping up a consistent work ethic. I found it incredibly hard to stay motivated - the typical second year blues, as I later heard them called. Throwing myself into a completely different environment made me understand how crucial teamwork is to me for maintaining my daily motivation, and this has made me reconsider my future career choices. I have learnt a great deal about how to effectively structure teams, plan work and communicate ideas across different teams throughout the company. Applying and developing these skills is what motivates me most at work.

Although I went into the internship hoping to learn more about data science, I ended up on the path of becoming a product manager - a role I had never even heard of before. Being exposed to the inner workings of an AI startup, from sales through product and project management down to different types of technical work, opened up a whole new world of previously unconsidered, potential career paths. The startup environment can be flexible, allowing you to try aspects of a variety of roles and stretching your comfort zone. For example, I even ended up going to two customer meetings. This experience has also reassured me that I do not need to know exactly what job I want to have in the next three, five or ten years - as long as I am learning skills that are important to me, I am on the right path.

My internship at Cytora was a great adventure of self-discovery. The experience has helped me really understand how to think about my personal development and has set me off on a great path for planning my future career. If you have the opportunity to apply your skills in another environment - take it, you never know what you will learn!

Epitomising the start-up environment. Left: Alise's favourite spot to work in the office. Top right: The Cytora team underneath blue Tenerife skys from a recent team trip. Bottom right: At a client launch party for insurance company QBE. (Image credit this page: A. Virbule; page facing: Materials studio screenshot Dr. V. Milman; simulation snapshots Biovia data sheet).

# A Unique Paradigm of Computational Research

Enter the surprisingly varied world of IBM Research with **Eduardo Ramos Fernandez**

Many people before me have written extensively about the wonders of doing an internship whilst doing a PhD. I am not going to do so. I just want to highlight that a break away from the PhD routine and the experience of going to the real world, away from the safe and comfortable environment one is accustomed to at university, is enriching - not to mention it always looks good on your CV! Instead, I will share with you my impressions on how IBM Research UK, where I was an intern for three months, works as a private scientific computing research organization.

The Daresbury IBM Research team in the Agile Working Laboratory. (Credit: K. Reusch)

IBM Research UK's headquarters are located within Sci-Tech Daresbury. This is a National Science and Innovation Campus close to Liverpool and Manchester where STFC scientists and private companies intertwine to push the boundaries of science and technology. This environment provides IBM Research with the ideal framework to implement a very interesting paradigm for computational scientific research based on a multi-disciplinary approach. Disciplines closer to Computer Science, such as machine learning, AI and data science are combined with physical modelling at different scales (from fluid dynamics and thermal analysis to atomistic modelling).

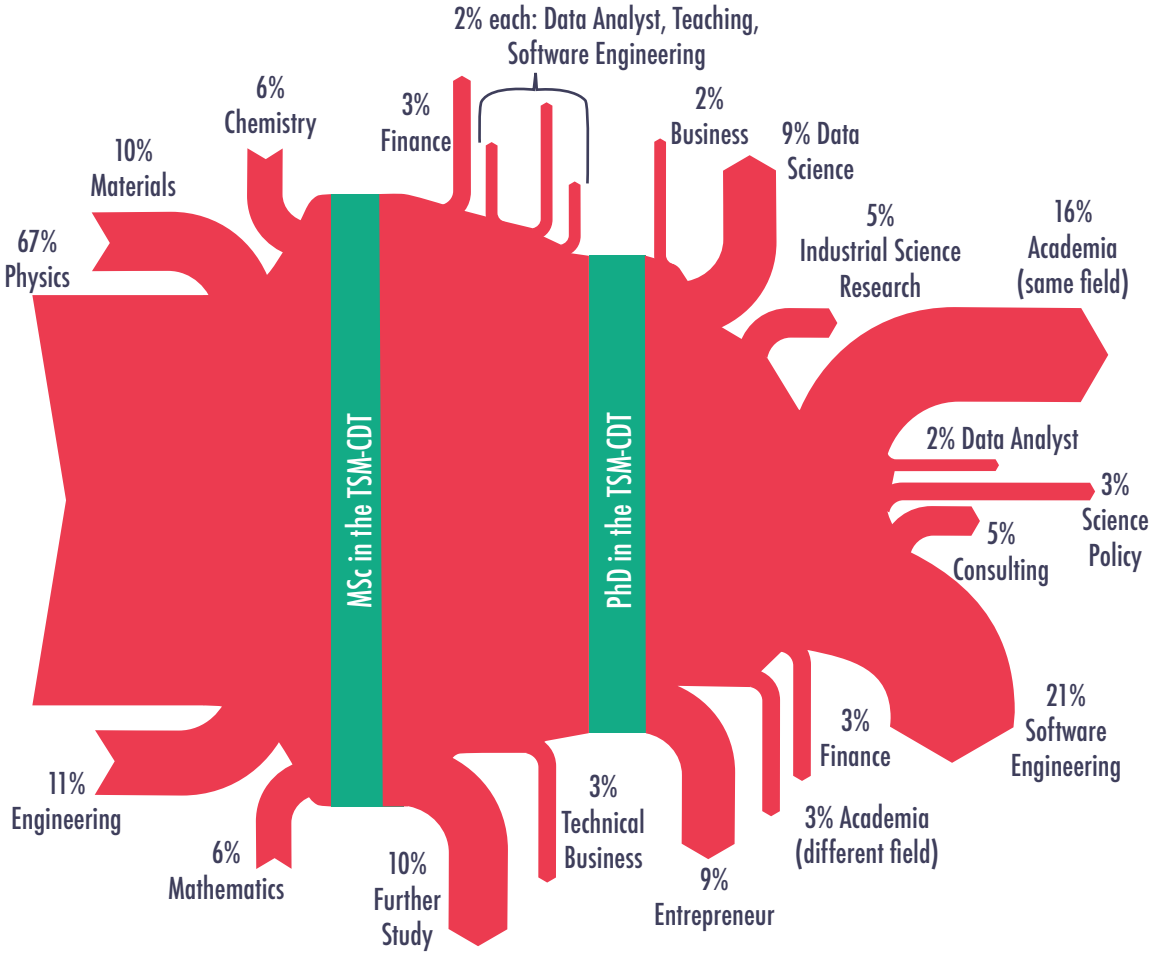
The research group is organized as an amalgam of small teams (4-6 people), each one bringing expertise from different fields. We can find the Engineering team (doing CFD, FEM analysis, optimization, ...), the Chemistry team (molecular, ab-initio and meso-scale methods), the Artificial Intelligence team, the Data Science team and finally some scattered computer scientists with expertise in compilers, parallel and distributed programming or systems administration. These groups, despite being mostly independent entities in terms of project management and leadership, usually cooperate together. The high crossover between the teams favours the permeability of expertise and knowledge throughout the whole research group. It is truly a luxury to always have one expert door-to-door who can help you from "why is my GPU code not working on the HPC using the gcc compiler?", going through "what would be a good artificial network topology to optimize my CFD mesh?" to "why is this not a good model to simulate supercooled liquid water at -10°C?". It is obvious that it is quite difficult for just one individual to accumulate all this know-how, but not if the research group work as such itself.

Moreover, the group benefits from weekly internal and external research seminars and courses, group activities to boost team working, and spare time for self-development. I found all of this quite refreshing. The weekdays are very dynamic as a result, and you get to know and share with different people in the group who you would otherwise not get the chance to see.

To sum up, the combination of expertise in HPC, Artificial Intelligence, Data Science and Scientific Computing (all in one place) to tackle real life industrial problems, really is the way forward in the broad field of applied computational research. On the other hand, this interesting scheme would be much more difficult to implement at the academic research level. Since, in the case of academia, the expertise is usually scattered across different, large research groups belonging to even different departments which make the collaborations difficult and slow to happen. The TSM-CDT aims to overcome this and to facilitate an interdisciplinary environment and collaboration. However, there is perhaps more to be done in this regard... But maybe that is a matter for another day!

# Life Beyond

*Explore the flow of students through the TSM-CDT Machine*




Input → Output

## ...and during: *CDT Prizes 2017-18*

The Sutton Prize for the best overall performance in the TSM MSc: *Zachary Goodwin*

The Materials Design Graduate Research Prize: *Lara Roman Castellanos*

The Materials Design Advanced Graduate Research Prize: *Iacopo Rovelli*

Johnson Matthey PhD prize winner: *Beth Rice and Nicola Molinari*

The Julian Walsh Prize for Outstanding Contribution to the Life of the TSM-CDT: *Andrew Warwick*

Major Contribution to the Life of the TSM-CDT: *Jana Smutna and Alise Virbule*

Outstanding Contributions to Outreach and Public Engagement: *Fangyuan Gu and Lara Roman Castellanos*

# Now that you're a Dr...

## Catch up with 3 recent Alumni

CW from top left: Boston skyline, basketball and New England hikes as Nicola enjoys PostDoc life. Andy giving an ML talk in home town Glasgow.

### Nicola Molinari

### PhD: Towards a predictive model of elastomer materials

**What's been next for you post PhD?**

I'm a Postdoctoral Fellow at Harvard. My current group works at the intersection of fundamental physics of materials properties, and data-intensive informatics approaches. I focus on accelerating discovery and design of new practical materials for breakthroughs in energy storage and conversion systems.

**How different is your current research area compared to your PhD?**

I would not say I work in a similar area as my PhD, as I mainly investigated the mechanical properties of polymer nanocomposites, yet I can apply a lot of the concepts that I learned. For instance, thanks to their tunable properties polymers are seen as attractive candidates to replace today's liquid electrolytes, consequently, I find the soft-matter expertise I developed throughout my PhD really useful. More generally, the most valuable and

### Andy McMahon

### PhD: The behaviour of charged species in hybrid organic-inorganic perovskite photovoltaics

**What has followed becoming a Dr?**

I've had two jobs, the first as "Head of Data Science and Machine Learning" at a Glasgow startup, and the second as a Senior Data Scientist at Aggreko, a world-leading mobile generator company. Essentially, I've gone wholeheartedly into the world of machine learning and AI!

**Did you have any prior idea what being a data scientist was like and why did you choose that route?**

I knew about half way through my PhD that I probably wouldn't be cut out for academia. I think academia requires you to focus on a very narrow area of science for large chunks of your career, and this didn't appeal to me since I'm pretty much curious about everything!

The more I researched and considered careers, I saw the 'Data Scientist' tag pop up again and again. After investigating, I realised that I could combine all the things I really enjoyed doing: mathematics, coding, solving practical problems, communication, and learning, into one career. I wouldn't be 'pigeon-holed' and could use my skills in any domain. I set about teaching myself the basics of data science and machine learning, which meant many evenings spent playing with Python code and reading articles and blog posts. The more I read the more that I knew that data science would be right for me, and I'm happy to say that after working in the domain for a few years that I've definitely made the right choice.

**Your career is quite different from the PhD, how much have you had to learn on the job?**

Although the raw technical skills are different, there is, in fact, a lot of overlap. My PhD involved running simulations where the aim was to minimise some function or functional. For example, in DFT we work to minimise the energy functional using gradient descent methods. Machine learning is actually the same type of problem, only now you are aiming to minimise your error or 'loss' to try and build an increasingly correct representation of the data.

I've definitely had to push hard on my coding and knowledge of specific algorithms, but you can do this on the job. Skills from my PhD, like learning quickly, logical reasoning, and to be comfortable solving tough problems, have been useful for doing this.

**Finally, top tip for anyone writing up?**

Keep going! Remember that you know what you are talking about and that you can write confidently and with authority about your topic. This also applies to your viva.

transferable skill I learned is to be efficient at learning and adapting different techniques that might better fit the technologically-relevant investigations I am pursuing.

Real-world problems are complex and intricate. As a result, I think that computational scientists like us should be open-minded, adaptable, and willing to often step out of the comfort zone of our favourite modelling technique, for instance.

### What's the contrast like between the role of a PhD student and stepping up to being a Postdoc?

My transition was pretty smooth, but I think there are a couple of differences. Firstly, you can impact more projects as more people look to you for answers. As a Postdoc, you have your own interest that you pursue, but you end up investing a lot of time consulting for other projects too. You start to become the point of reference for a class of questions, which takes you in all sorts of interesting directions.

A flip side to this, is that you have more responsibilities, both scientifically and organisationally. You can easily end up mentoring a PhD student and feeling responsible for the student's scientific and personal development. Additionally, you start engaging with CV screenings, grant proposals, general group maintenance and so on. I enjoy both aspects, as you end up learning unexpected things and they are useful opportunities for both my own and others development.

### How is life at Harvard and in Boston compared to Imperial and London?

I really love Boston! I enjoyed living in London, but I was ready and happy to try a new adventure. The environments are pretty comparable between Harvard and Imperial. If I have to find something, I would say Harvard is more culturally diverse. I think this stems from the fact that Harvard is not a pure science and technology university, resulting in a campus rich in events and opportunities in other fields.

### Any plans for the next 6 months or beyond?

...Work?!

## Freda Jaeger

## PhD: Flow of fluids through porous media with application to membranes: from the molecular to the continuum scale

### Since finishing your PhD what have you been up to?

I went on a 5.5 week holiday to southeastern Europe (7 countries!) before starting my new job.

### Had you always planned to travel after finishing?

No, I thought I would go straight into a job, or take some time to visit family. I'm really glad I went away though as it was great to give my brain a break and normally, you don't get the opportunity to easily take 6 weeks off work. Plus, I would've never applied to my current job without the break and having some time to consider what I actually want from my career.

### From your travels, what was your favourite country?

Bosnia and Herzegovina, although I only went to Sarajevo, Mostar and the surrounding area there's a great mix of beautiful landscapes and interesting (albeit depressing) history. The people there are super friendly and really keen to share their experiences and opinions of the country. I learned so much just from speaking to people and you can really tell that they still like visitors. Plus, it's cheap!

### What is your new job and how is it different to PhD life?

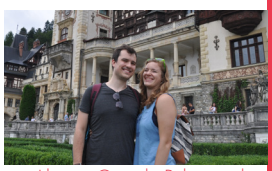
I'm a back-end software engineer at Octopus Energy, who focus on providing renewable energy. It's a small and tech-focussed energy company with a great relaxed atmosphere. The main difference to PhD life is that you achieve things on small time scales which is very satisfying. There's so much to learn about the world of software engineering but you pick things up quickly and can make a meaningful contribution after a very short time. The other great thing is that you can actually just stop thinking about work when it's the weekend/holidays (no guilt!).

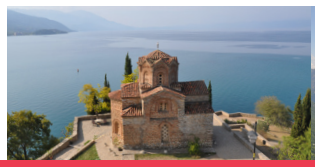
### What was the largest challenge during your PhD and how did you get past it?

Staying motivated, it seemed like I had no idea what I was doing and everything I tried wasn't working. I basically moved on from things that I thought were never going to work out and did a lot of reading on the rest until I finally knew what was happening and what I had to do. It took a long time though!

### Finally, top tip for anyone writing up?

Start early. I started a year before I submitted and I wasn't under pressure at the end at all. Work on the methods/theory early on, it might even help you understand what you're doing.



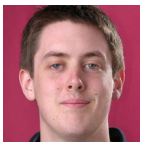


Above: Outside Peleș castle, Romania; Below: shots from Macedonia and Albania

# TSM-CDT Students and Research Projects

## Cohort VI

**Chris Ablitt -** First Principles Lattice Dynamical Study of Ferroelectric and Negative Thermal Expansive Rud-dlesden-Popper Oxides
*Prof. Arash Mostofi (Mat/Phys), Dr Nicholas Bristowe (Kent), Dr Mark Senn (Warwick -Chem)*



**Robert Charlton -** Computational Excitonics of Doped Organic Molecular Crystals for a Room Temperature Maser (ICL PhD Scholarship)
*Prof. Peter Haynes (Mat/Phys), Prof. Andrew Horsfield (Mat)*

**Jacek Golebiowski -** Polymeric CNT Composites – Atomistic Simulation of the Effects of CNT Functionalisation on Inter-facial Properties (Marie Skłodowska-Curie European Training Network co-funded)
*Prof. Peter Haynes (Mat), Prof. Arash Mostofi (Mat/Phys)*

**Eduardo Ramos Fernández -** Mul-ti-Scale Modelling of Hydrodynamic Lubrication and Friction (BP funded)
*Prof. Daniele Dini (Mech Eng), Prof. David Heyes (Mech Eng)*

**Gleb Siroki -** Optical Properties of Topological Insulator Nanoparticles
*Dr Vincenzo Giannini (Phys), Dr Derek Lee (Phys), Prof. Peter Haynes (Mat/Phys)*

**Alise Virbule -** Design of High Absorp-tion Organic Semiconductors for Appli-cations to Solar Cells and Light Emission
*Prof. Jenny Nelson (Phys), Dr Johannes Lischner (Mat)*

**Ignacio Bordeu -** Theory of active matter (Conicyt funded)
*Dr Gunnar Pruessner (Maths), Prof. Henrik Jensen (Maths)*

**Lars Blumenthal -** Electronic Excitations at Solid-Liquid Interfaces: Combining Many-Body Perturbation Theory with Molecular Dynamics Simulations
*Dr Paul Tangney (Mat), Dr Johannes Lischner (Mat)*

**Luca Cimbaro -** Embrittlement of Ni-based Superalloys by Oxygen (Rolls-Royce funded)
*Dr Daniel Balint (Mech Eng), Prof. Tony Pax-ton (KCL - Phys), Prof. Adrian Sutton (Phys)*

**Hikmatyar Hasan -** Designing Next Generation High-Temperature Co-Al-W Based Superalloys
*Dr Vassili Vorontsov (Mat), Prof. Peter Haynes (Mat/Phys), Prof. David Dye (Mat)*

**Iacopo Rovelli -** High Temperature Loss of Strength in Ferritic/Martensitic Steels for Fusion Energy Applications (Culham Centre for Fusion Energy funded)
*Prof. Adrian Sutton (Phys), Prof. Sergei Dudarev (Phys)*

**Jonas Verschueren -** Fundamentals of Dislocations in Motion
*Prof. Daniele Dini (Mech. Eng.), Dr Daniel Balint (Mech. Eng.), Prof. Adrian Sutton (Phys)*

**Marise Westbroek -** Flow in Porous Media (Janet Watson scholarship)
*Prof. Peter King (Earth Sci & Eng), Prof. Dimitri Vvedensky (Phys)*

## Cohort VII

**Harry Cárdenas -** Molecular thermo-dynamic models for adsorption
*Prof Erich A. Müller (Chem Eng)*

**Fangyuan Gu -** First Principles Lattice Controlling structural change in multiferroic materials by ultrafast laser excitation
*Dr Éamonn Murray (Mat), Dr Paul Tangney (Mat)*

**Nuttawut Kongsuwan -** Strong Coupling in Plasmonic Nanocavities (ICL and Thai Government funded)
*Prof. Ortwin Hess (Phys)*

**Nikoletta Prastiti -** Modelling methodologies for microstructure-sensitive crack growth in aero-engine PM Ni alloys
*Dr Daniel Balint (Mech Eng), Prof. Fionn Dunne (Mat)*

**Christopher Sewell -** Advancing the atomistic theory of corrosion passivation in sulfidic environments (BP funded)
*Prof. Nicholas M. Harrison (Chem)*

**Andrew Warwick -** Emergent Phenomena at domain walls in halide perovskites
*Dr Nicholas Bristowe (Mat), Prof. Peter Haynes (Mat/Phys)*

**Martik Aghajanian -** Adsorbate engineering in two-dimensional semiconductors
*Dr Johannes Lischner (Mat) , Prof. Arash Mostofi (Mat/Phys)*

**Sophie Finnigan -** Modelling the decomposition of chemical warfare agents in the environment
*Dr Kim Jelfs (Chem), Prof. Patricia Hunt (Chem)*

**Syed Hussain -** Group theoretic methods for semi-empirical electronic structure of topological materials
*Prof. Dmitri Vvedensky (Phys), Prof. Jing Zhang (Phys), Dr Paul Tangney (Mat)*

**Mariana Hildebrand -** Towards the manipulation of defects and dopants to functionalise graphene
*Prof. Nicholas M. Harrison (Chem)*

**Charles Penny -** The contribution of surfaces to the magnetic Curie temperature and magnetic recording fidelity (STFC funded)
*Dr Adrian Muxworthy (Earth Sci & Eng), Dr Karl Fabian (NGU, Norway) and Prof Valera Shcherbakov (RAS, Russia)*

**Lara Román Castellanos -** Hot electrons in nanoplasmonics: combining quantum mechanics with nanophotonics
*Prof. Ortwin Hess (Phys), Dr Johannes Lischner (Mat)*

**Panagiotis Simatos -** The impact of combustion-generated moieties on the degradation of ICE related surface materials (Toyota Motor Europe funded)
*Prof. R. Peter Lindstedt (Mech Eng) , Prof. Daniele Dini (Mech Eng), Dr Konstantinos Gkagkas (Toyota Motor Europe)*

## Cohort VIII

**Cristian Constante Amores -** Multi-phase modelling of oil-water droplet size districations (BP funded)
*Prof. Omar Matar (Chem Eng)*

**Emanuele Galiffi -** Transformation optics applied to plasmons in graphene
*Prof. Sir John Pendry (Phys), Dr Paloma Arroyo Huidobro (Phys), Prof. Norbert Klein (Mat)*

**Samuel Palmer -** Simulation of phoxonic metamaterials
*Dr Vincenzo Giannini (Phys), Prof. Richard Craster (Maths)*

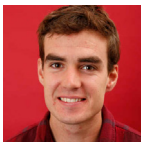
**Luca Reali -** Cyclic loading and delayed hydride cracking in Zr-alloys (Rolls-Royce funded)
*Prof. Adrian Sutton (Phys), Dr Daniel Balint (Mech Eng), Dr Mark Wenman (Mat)*

**Jana Smutna -** Understanding the role of hydrogen-dislocation interactions in the corrosion and hydrogen uptake of irradiated zirconium fuel cladding alloys (Rolls-Royce funded)
*Dr Mark Wenman (Mat), Prof. Andrew Horsfield (Mat), Prof. Adrian Sutton (Phys)*

**Tomos Wells -** Spin-lattice coupling in magnetic materials (Culham Centre for Fusion Energy funded)
*Prof. Andrew Horsfield (Mat), Prof. Matthew Foulkes (Phys), Prof. Sergei Dudarev (EURATOM, Phys)*

**Zainab Alaithan -** Theoretical characterisation of zeolites (Aramco funded)
*Prof. Nicholas M. Harrison (Chem)*

**Dimitrios Bikos -** Effect of structure on oral and industrial processing of aerated chocolate products (Nestle funded)
*Prof. Maria Charalambides (Mech Eng), Dr Marc Masen (Mech Eng), Dr Philippa Can (Mech Eng), Prof. Yannis Hardalupas (Mech Eng)*



**Zachary Goodwin -** Discovering twisted bilayer materials with strong electron correlation
*Dr Johannes Lischner (Mat) , Prof. Arash Mostofi (Mat/Phys)*

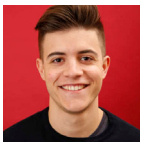
**Carles Rafols i Belles -** Multiscale modelling of corrosion scales (BP funded)
*Prof. Nicholas M. Harrison (Chem)*

**Rosemary Teague -** Modelling the impact of vibrational modes on electronic dynamics and transport in molecular electronic materials and devices
*Prof. Jenny Nelson (Phys), Dr Artem Bakulin (Chem), Dr Jarvis Frost (Phys visitor)*

**Marie Rider -** Quantum optics with topological insulator nanoparticles
*Dr Derek Lee (Phys), Dr Vincenzo Giannini (Phys), Prof. Peter Haynes (Mat/Phys)*

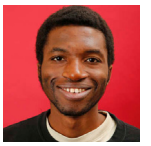
**Aliki-Marina Tsopelakou -** Reaction mechanisms for materials systems with complex potential energy surfaces (Toyota funded)
*Prof. Peter Lindstedt (Mech Eng), Prof. Daniele Dini (Mech Eng)*

## Cohort IX



**Carlos Ayestaran Latorre -** Unravelling the role of mechanochemistry in lubrication mechanisms (Afton funded)
*Prof. Daniele Dini (Mech. Eng.), Prof. Hugh A. Spikes (Mech Eng), Dr James P Ewen (Mech Eng)*

**Gabriele Coiana -** Strongly correlated phonons in ferroelectrics and perovskite superlattices
*Dr Paul Tangney (Mat), Dr Johannes Lischner (Mat)*



**Matthew Okenyi -** Mesoscopic size effects on organic ferrolectrics
*Dr Laura Ratcliffe (Mat), Prof. Aron Walsh (Mat)*

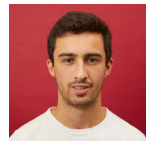
**Georgios Samaras -** Micro-mechanical model development for predicitng the effect of microstructure on bulk behaviour or aerated soft solids (Nestle funded)
*Prof. Maria Charalambides (Mech Eng), Dr Marc Masen (Mech Eng), Dr Philippa Can (Mech Eng), Prof. Yannis Hardalupas (Mech Eng)*

**Yiyuan (Amy) Wang -** Theory and simulation of charge injection at metal-polymer interfaces (ABB funded)
*Prof. Arash Mostofi (Mat/Phys), Dr Mikael Unge (ABB Corporate Research)*

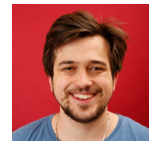
# Cohort X

Mohamed Adelbar
MSc Student

Christopher Bradley
MSc Student

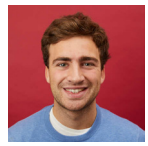


Christopher Keegan
MSc Student

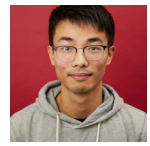


Martin Lazo
MSc Student

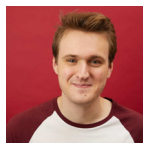
Puck Van Gerwen
MSc Student



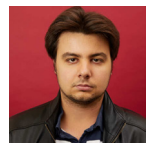
Michele Valsecchi
MSc Student
(P&G funded)



Kang Wang
MSc Student

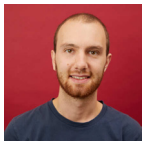


Thomas Yates
MSc Student

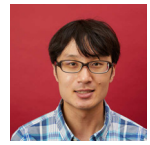


Christian Zagar
MSc Student

Mario Zauchner
MSc Student

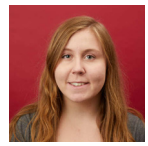


Matthias Kiesel - Direct PhD
From molecules to macrophases: Structural properties of ionic surfactant solutions (P&G funded)
*Prof. Amparo Galindo (Chem Eng), Prof. George Jackson (Chem Eng)*



Kazuki Morita - Direct PhD
Materials informatics of multi-component metal oxides (Yoshida Foundation Scholarship and Materials Dept. funded)
*Prof. Aron Walsh (Mat)*

Miriam Scharnke - Direct PhD
Ultrafast dynamics of excitons in 2D materials (RS funded)
*Dr Johannes Lischner (Mat), Dr Johannes Knolle (Phys)*



Emma Richards - Direct PhD
Viscosity and phase boundary predictions through coarse grained molecular modelling (P&G icase)
*Prof. Erich Muller (Chem Eng), Prof. George Jackson (Chem Eng)*

## TSM-CDT Staff

**Prof. Arash Mostofi** – *Director*
**Dr Johannes Lischner** – Assistant Director and Cohort 10 Mentor
**Prof. Peter Haynes** - Strategic Advisory Team
**Prof. Adrian Sutton** - Strategic Advisory Team
**Prof. Mike Bearpark** – Cohort 6 Mentor
**Prof. Andrew Horsfield** – Cohort 7 Mentor
**Dr Kim Jelfs** - Cohort 8 Mentor
**Prof. Daniele Dini** - Cohort 9 Mentor
**Dr Simon Foster** – Outreach Officer
**Miss Miranda Smith** – Senior CDT Administrator
**Miss Naho Ollason** - CDT Administrator

## External Advisory Board

**Dr Kate Bowman** - EPSRC Representative
**Prof. W Craig Carter** - Massachusetts Institute of Technology (MIT), USA
**Dr John Stevens** - Baker Hughes, UK
**Dr Dirk Dijkstra** - Covestro Deutschland AG
**Prof. Sergei Dudarev** - EURATOM Fusion, UK
**Prof. David Rugg** - Rolls-Royce, UK
**Dr Simon Schultz** - CDT Neurotechnology, ICL
**Prof. Dr Helena Van Swygenhoven** - Paul-Scherrer Institute & EPFL, CH
**Dr Erich Wimmer** - Materials Design, USA
**Prof. Ellen Williams** - University of Maryland, USA

## Contact details

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Web: www.tsmcdt.org

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Imperial College London
Exhibition Road
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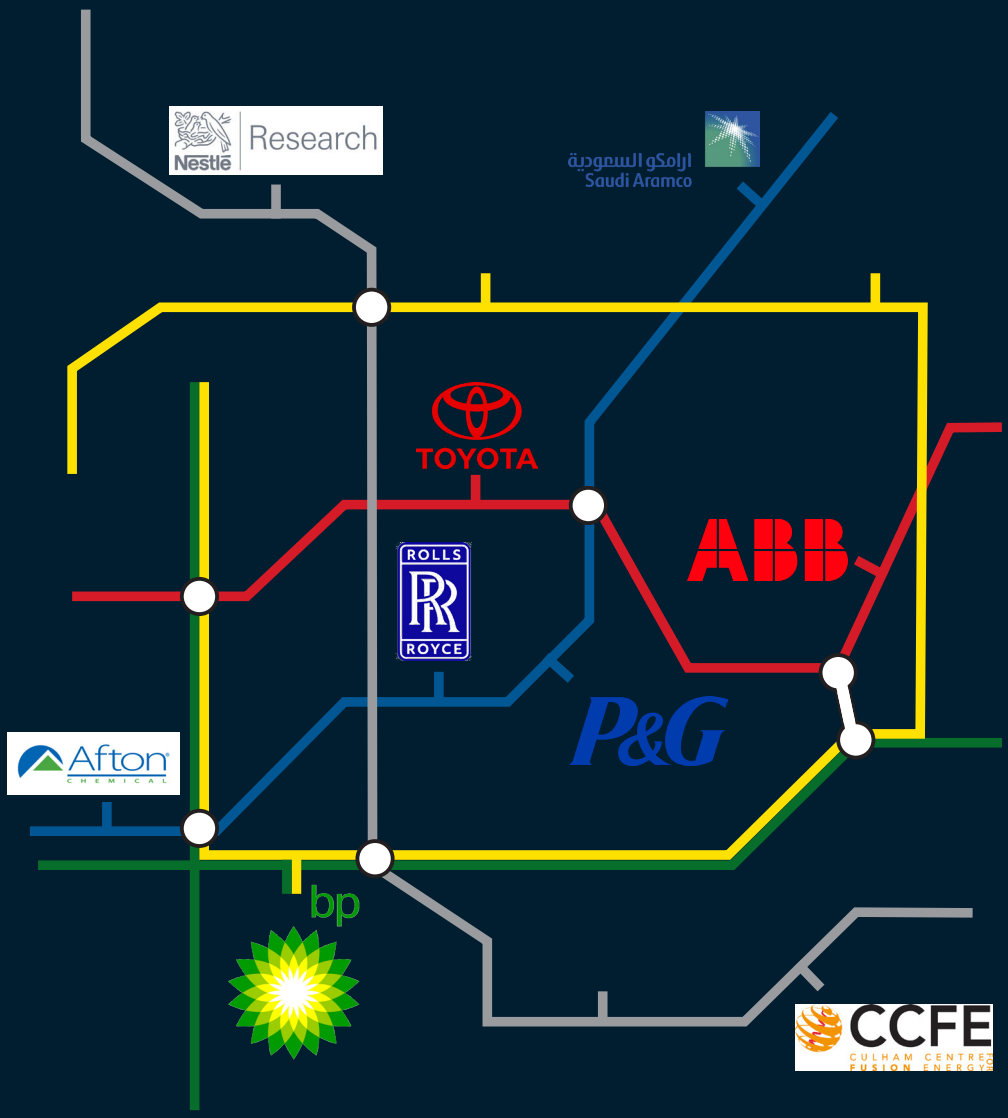
**Code For Creation defect puzzle answers:**

1. Thomas
2. Atomic
3. Metals
4. MEACEC
5. Scales
6. Length

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