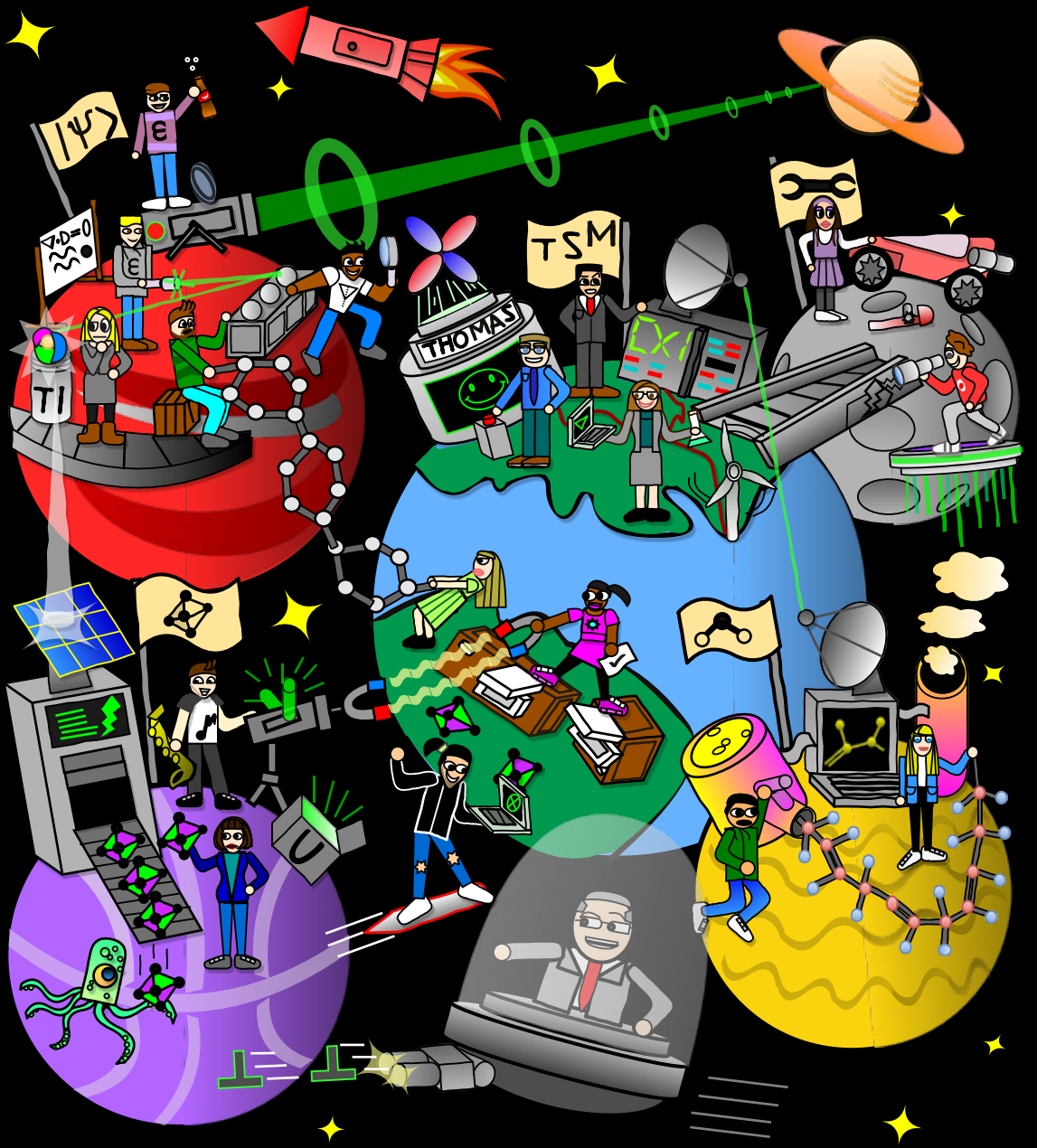
Annual Report

Centre for Doctoral Training in Theory and Simulation of Materials



2016-17

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We would like to acknowledge the work of the editors from previous years, particularly Chris Ablitt and Alise Virbule, for an excellent template and advice.

London, November 2017

'If it wasn't hard, everyone would do it. It's the hard which makes it great'.

- Tom Hanks

Contents

Meet the CDT
Director's Foreword

This year we welcomed our ninth cohort of students to the TSM-CDT, taking the total number admitted since we opened our doors in 2009 to over 100. This centuria of students is at the heart of our central mission to create a new generation of scientists and engineers with the theoretical and computational abilities to model properties and processes within materials across a range of length and/or time scales. In doing so, we also aim to create an environment in which students are able to flourish more broadly to become valuable members of society. In other words, the philosophy of the CDT is to couple a deep technical training with a strong emphasis on personal development.

Technical training begins with the MSc in year 1, in which students learn the theory and computational tools associated with the different scales and think about what is involved in bridging them. In their PhDs, they work with supervisors and collaborators whose expertise resides at different scales and they gain direct experience of the approach associated with the different scales and work on how to bridge them. This experience not only equips them with domain-specific knowledge and skills, but with a host of associated skills (critical thinking, communicating complex ideas, and team-working to mention but a few) that they can put to use, whatever their chosen career (see pages 26-27).

Personal development is fostered through a suite of activities, many of which you will read about in the pages that follow (which, incidentally, have been entirely written and edited by students). A particular highlight of the year has been the success of our students in the Imperial College President's Awards for Excellence in Societal Engagement. Two out of the five annual awards made across the entire College were won by CDT students. One went to Beth Rice (cohort 5) who is the founder and organizer of a Science Club for girls aged 6 to 11 that runs at the Baytree Centre in Brixton. This is a charity that was set up during the social unrest of the 1980s as a safe space for girls and women to develop socially and educationally. Through her work, Beth is supporting, encouraging and educating girls from some of the most disadvantaged neighbourhoods and schools in south London. Another award went to Chris Ablitt and Rob Charlton (cohort 6) who were the key organisers of the "Atoms to Galaxies" series of the Pint of Science Festival. Pint of Science is an annual event that aims to bring cutting-edge research to the public in an accessible format and in the relaxed atmosphere of a pub. Chris, Rob and their team attracted sell-out crowds of over 100 people every night it ran.

These are but two examples of the many and varied ways in which our students engage with society. Each and every one of these interactions is an immensely valuable contribution that helps sow the seeds of logical and scientific thinking in society, arguably the bedrock of future prosperity. It is a source of great pride that so many of our students are involved in such activities – they are a great credit to the CDT and to the College.

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

A Whirlwind Tour
Cohort 8's MSc Year

On a surpringly warm September day, 15 strangers were bundled into the Whiteley Suite with names on handwritten labels, ready to embark on 12 months they'd never forget...

START

Physics - *Imperial College London*
Theoretical Physics - *Cambridge University*
Industrial Engineering - *Univeristy of Trento, IT*
Materials Science and Engineering - *University of Ioannina, GR*
Perimeter Scholars International MSc - *Perimeter Institute for Theoretical Physics, CA*
Physics - *Jilin University, CH*
Natural Sciences - *Lancaster University*
Physics - *National and Kapodistrian University of Athens, GR*
Physics - *University of Rochester, USA*
Advanced Chemical Engineering MSc - *Imperial College London*

COURSES

And so began an intense but thorough training spanning scales and disciplines.

Transformations of Materials

A truly multi-scale approach to the formation of microstructure in materials and its effect on material properties, from the atomistic nature of diffusion to the effect of heat treatment on alloys.
Jana Smutna

Mathematics for the Theory of Materials

A broad selection of mathematical techniques for modelling materials, with something new for everyone.
Sam Palmer

Classical Field Theory of Materials

Even after 5 years of engineering I found this module extremely interesting. The theory of planar elasticity in the language of complex analysis is elegant and invaluable knowledge for my PhD.
Luca Reali

Group Research Strategy Project

An absolutely unique course on writing an academic proposal. The writing skills, panel interview, and the approach to breaking down the problem are some of the most useful skills I learnt and developed during the MSc.
Sophie Finnigan

A really valuable introduction on how to approach a research problem where the answer is unknown, but you still have to devise a route to the solution. Planning how to solve a problem over 2-3 years rather than 2-3 hours is quite the paradigm shift.
Marie Rider

Above: One GRSP group visiting NPL and Left: Champagne means results celebration!

Electronic Structure of Materials

As a physicist, this was a good reminder of the key concepts in condensed matter theory that I needed for my project, namely tight-binding and density functional theory.
Martik Aghajanian

Equilibrium in Materials

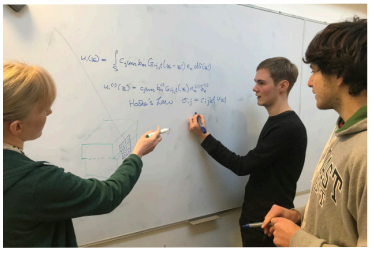
A thorough approach to the subject of thermodynamics, covering concepts needed by physicists to explain the behavior of real world materials, such as phase diagrams. EQM complimented the other courses well, providing a macroscopic angle on phenomena we had been introduced to from a more atomistic perspective.

Tomos Wells

Methods of Simulating Materials

A mini safari tour of different simulation methods. It provides you with knowledge of the range of tools out there and the scales at which they're suitable. Being given example codes to play with gives you experience you wouldn't gain using 'black box' software.

Sophie Finnigan



Left: Collaboration is the key to MSc survival..., Below: ...and so is food!

Computational Methods

This course helped us practice and build on our coding skills while introducing important numerical methods. The final project let us explore a topic in depth and get more familiar with version control as a cooperation tool.

Jana Smutna

SOCIAL

Mentor lunches every week, collaboration on problems and social plans outside bonded us as a cohort and saw us all through. While organising the annual Christmas party and Summer BBQ and football (see page ...) integrated us into the rest of the CDT.

Never a dull moment. The comprehensive workload means that the student organisers are determined to make the social events as fun as possible.

Martik Aghajanian

I will always remember opposing feelings of wondering whether I would be able to cope with something while being certain that I was good at something else. But what makes them sweet memories is that I always found someone ready to help me or that I could help. The MSc experience teaches a lesson on help: the importance of both seeking for it, and being willing to offer it.

Luca Reali

The cohort structure provides a ready made support network and you get the most out of the course if you use it. The more I started to ask others for help the more I learnt. Sometimes it feels like you're the one asking all the questions, but our academic backgrounds are so diverse that there comes a time when you're able to give back.

Sophie Finnigan

FINISH

MSc Alumni	Chem. Eng.
Materials	Physics
Mech. Eng.	Mathematics
Chemistry	...and all firm friends!

Life in the CDT

During your TSM-CDT experience what's been the biggest challenge?...

Not to die by deadlines!

Eduardo Ramos Fernandez (Cohort 6)

The taught MSc is definitely the toughest part. We all come from different backgrounds and in the MSc we face problems on topics that we've never encountered before. Thankfully, everyone's really smart and helpful, so if you don't know there's someone willing and able to lend a hand. Juggling everything I had to do wasn't easy but was very rewarding and excellent preparation for the PhD.

Rob Charlton (Cohort 6)

Keeping going when nothing is working and you have no idea what you're doing.

Frederike Jaeger (Cohort 5)

To stop thinking like an undergrad: trying to understand all the cool stuff other people have done, and to start thinking like a researcher: thinking up cool things to do which have never been done.

Chris Ablitt (Cohort 6)

Because of the multi-disciplinary nature of the course it was a challenge for people from different backgrounds to communicate at first. For example, coming from an engineering background and approaching a more physics based understanding.

Angeliki Poulou (Cohort 8)

Above: Enjoying the taste of graduation
Bottom left: Smiles all round at the TSM annual conference

...and what's been the highlight?

Definitely the variety of people and opportunities that I have been exposed too.

Nicola Molinari (Cohort 5)

Getting a paper published in Nature.

Peter Fox (Cohort 5)

The people I get to interact with, both from my cohort, other cohorts and the academics and people from industry that come to speak to us.

Jana Smutna (Cohort 8)

Organising the CDT Annual Conference.

Luca Cimbaro (Cohort 6)

Alternative meaning for TSM?

Thanks, Seriously, to Miranda

Chris Ablitt (Cohort 6)

The Science Menagerie

Anthony Spice (Cohort 8)

Totally Super, Man!

Peter Fox (Cohort 5)

What do you think is the biggest strength of the TSM-CDT?

Small class sizes (during the Masters) and proximity to world class academics.

Anthony Spice (Cohort 8)

It isn't just a regular PhD. We're challenged to try lots of different things regardless of background, or whether we really want to! Be it programming in a team, explaining our reserach to the general public, making a radio show, or organising the Christmas party, it all adds up to a great experience.

Rob Charlton (Cohort 6)

Providing students with a grounding in programming.

Gleb 'the group programming project' Siroki (Cohort 6)

Without the CDT there is no way we would know so many people working in so many different areas of materials models with whom to: bounce ideas off, share expertise, drink coffee and solve problems with.

Chris Ablitt (Cohort 6)

Collaboration.

Emanuele Galiffi (Cohort 8)

Above: Gowned and crowned Doctors
Middle-right: The TSM party warms up

What would you say to your younger self who was thinking about applying to the TSM-CDT?

It's a great opportunity to get into a PhD programme where you're sure that someone cares about you!

Emanuele Galiffi (Cohort 8)

Do it, do it! (Whispering...)

Eduardo Ramos Fernandez (Cohort 6)

Prepare for some tough years but it will all make sense in the end.

Frederike Jaeger (Cohort 5)

Run (to it), you fool!

Nicola Molinari (Cohort 5)

How well has the TSM-CDT experience prepared you for life after your PhD?

Pretty well from what I can tell, especially in terms of confidence from taking on projects outside of your PhD.

Frederike Jaeger (Cohort 5)

It has allowed me to drive my PhD project in a different direction, which has equipped me with extra skills that open up more job opportunities.

Charlie Penny (Cohort 7)

The programme encouraged teamwork and trained students to deal with tight deadlines.

Angeliki Poulou (Cohort 8)

Credit: E. Galiffi

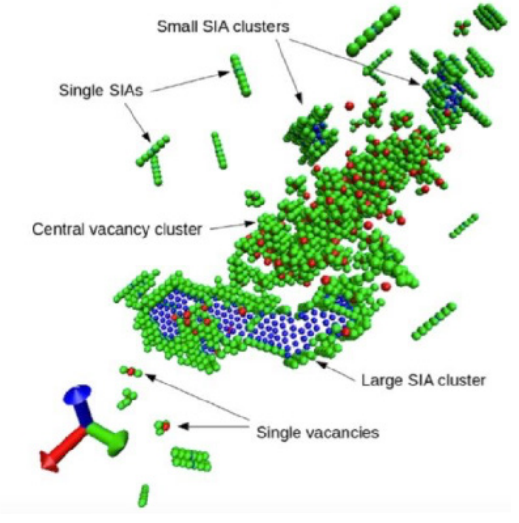
Research Highlight

Non-local Model for Diffusion Mediated Dislocation Climb and Cavity Growth

Iacopo Rovelli summarises his research into modelling radiation defects.

Achieving energy production via nuclear fusion reactors is one of the most scientifically and technologically demanding tasks of our time. In the future, fusion power will be a fundamental tool in order to meet the growing global energy demand, while reducing CO_2 emissions. The most promising (and heavily funded) design paradigm involves tokamak reactors: massive toroidal-shaped machines that magnetically confine plasma heated to millions of degrees in order to spark the fusion of deuterium and tritium nuclei.

While a considerable amount of research has been aimed at understanding plasma dynamics in a fusion reactor, another important area of research involves design of structural materials (mainly tungsten, beryllium and steel alloys) able to withstand the extreme conditions of the reactor. High energy neutrons from the fusion reaction displace atoms from their equilibrium positions, leading to collision cascades (Fig) that generate free vacancies and interstitials, which then coalesce into nanometric defect clusters.



Post-irradiation annealing is a promising route for the maintenance of structural materials in next generation tokamak reactors. Therefore, precise quantitative knowledge of the annealing timescales of radiation-induced defects is needed.

During my project, partially funded by EURATOM, I've developed a new method in order to predict annealing timescales for arbitrary configurations of radiation defects, in collaboration with Prof. Adrian Sutton and Prof. Sergei Dudarev from the Culham Centre for Fusion Energy. It turns out that the problem is mathematically very similar to a system of interacting charges in electrostatics. Therefore, some of the techniques developed in that context can be easily adapted. Numerical results in the simplified case of a dilute configuration of prismatic dislocation loops and spherical cavities show a good agreement with experimental data on defect annealing in ion-irradiated tungsten. This was achieved using only physical parameters as inputs for simulations, with no parameter fitting.

We are currently working on an extension of the model in order to treat experimentally unobservable clusters as an effective mean field coupled with the evolution of discrete clusters. This will help us to inform future experimental investigations and to explore more efficiently wide ranges of defect distributions.

Fig: Defect configuration resulting from a simulated collision cascade
Credit: Sand, A.E., Nordlund, K. & Dudarev, S.L., 2014, 455(1-3), 207–211

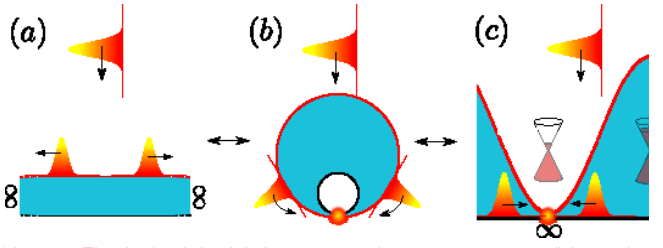
For more details see: I. Rovelli, S. L. Dudarev, A. P. Sutton, J Mechan Phys Solids, 103, 121–141, 2017

Research Highlight

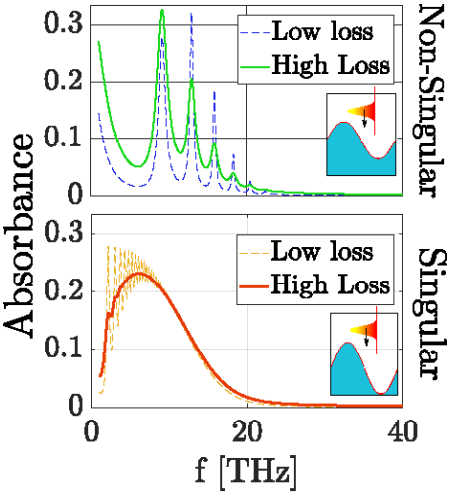
Hidden Dimensions in Singular Graphene Metasurfaces

***Emanuele Galiffi** talks about his recent work on graphene and transformation optics.*

Advanced field theories hypothesise the existence of more than four dimensions, the extra dimensions described as compacted into unmeasurably small length scales. In our work on singular plasmonic structures[1], we reported the phenomenon of hidden dimensionality in a simple plasmonic metasurface, which may be designed on graphene by spatially modulating its Fermi level with a grating profile, such that the charge carrier density is strongly suppressed at one point.



Above: Fig 1: A slab (a) is mapped to a crescent (b) and a grating (c), realised as a periodically doped graphene sheet. In (a) waves travel towards infinity, which is mapped onto the singularity in (c).



Right: Fig 2: The discrete absorption spectrum of a conventional grating (top) becomes continuous for a singular one (bottom).

As opposed to conventional gratings, which are characterised by two wave vectors, this metasurface is effectively described by three, the extra wavevector being inherited from the hidden dimension and not fixed by the incident radiation. The presence of this extra degree of freedom implies that the necessary phase matching for the excitation of surface plasmons can be achieved for a broad frequency band, as opposed to a discrete set of resonances. As a result, the surface plasmon resonance frequencies are squashed into a continuum of modes, which can be efficiently coupled to incident radiation.

Transformation optics enabled us to elegantly illuminate the physics at play: we used a conformal map to relate a singular grating to a spectrally equivalent, translationally invariant slab, (Fig 1). Conformally approaching the singular limit amounts, in the slab frame, to quantising the modes over a unit cell whose width tends to infinity, meaning that the Brillouin zone size is shrunk to zero, thus the resonance frequencies merge into a continuum.

This feature of singular gratings enables the design of strong broadband THz absorbers on atom-thick layers[2], whose frequency may be tuned via the grating periodicity. Remarkably, these devices are able to excite a wealth of high order plasmons, achieving extreme subwavelength confinement of the incoming THz light, (Fig 2). Our results promise to open a new direction in the current technological race towards the manipulation of THz radiation.

1: J.B.Pendry, P.A.Huidobro, Y. Luo, E. Galiffi, Science, 358 (6365), 915-17, 2017

2: E. Galiffi, J. B. Pendry and P.A. Huidobro. ACS Nano - submitted.

Credit: L. Blumenthal

Research Highlight

Energy Level Alignment at Semiconductor-Water Interfaces

Lars Blumenthal summarises his work on atomistic and continuum simulations of semiconductor-water interfaces.

The grand idea of photoelectrochemistry is to harvest the energy carried by sunlight and to directly convert it into chemical energy, i.e. energy stored in the form of chemical bonds. This could provide a clean and sustainable source of fuels or important chemical feedstocks. To achieve this, one could connect a photovoltaic device to an electrochemical cell; the former would harvest the solar energy and the latter would convert it into chemical energy. However, a far more elegant solution is to combine both devices into one so that the semiconductor that absorbs the incoming photons also acts as an electrode at whose surface the desired redox reactions take place (Fig).

This concept was first realised by Fujishima and Honda in 1972[1] and has since sparked an enormous research effort with the objective of increasing the efficiencies of these photoelectrochemical cells. Unfortunately, a semiconductor immersed in an electrolyte constitutes a far more complicated system than one might initially think and so progress has been slow.

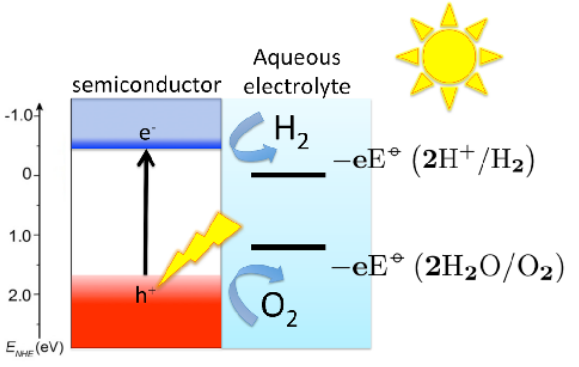


Fig: Depending on the position of the band gaps, the excited electrons and holes can drive reduction and oxidation reactions at the semiconductor's surface.

Computational modelling might aid the development of these devices by screening for more suitable semiconductors or by revealing insights into the underlying physical processes occurring in a working photoelectrochemical cell. However, building a realistic theoretical model of the semiconductor-electrolyte interface, which forms the central part of this technology, is extremely challenging. In particular, simply using density functional theory (DFT) for the semiconductor's electronic structure is often not good enough as the absolute position of the electronic band edges, something DFT cannot really predict very well *a priori*, is an important descriptor. Furthermore, determining the atomic structure of the interface usually requires *ab initio* molecular dynamics (AIMD) as classical force fields usually lack transferability or are not available to begin with.

In our recent paper, we developed a workflow that merges two existing methods to reduce the computational cost of simulating the semiconductor-electrolyte interface while still maintaining an appropriate level of accuracy[2]. The workflow employs the GW formalism for the semiconductor's electronic structure and a continuum model to describe the electronic response of the electrolyte. We demonstrated that our approach compares well with the combination of GW and AIMD, and are now looking forward to exploiting this to simulate the interface in an electrochemically more realistic state.

1. A. Fujishima and K. Honda, Nature, 238, 37, 1972
2. L. Blumenthal et al, RSC Adv., 7 (69), 43660-43670, 2017

Research Highlight

Dislocation Injection: Bridging the Atomistic-Continuum Scales

Jonas Verschueren ***on his work investigating fast moving dislocations by atomistic simulations.***

Dislocations travelling at speeds comparable to the speed of sound in a material occur under shock-loading conditions. However, the physics associated with these fast-moving dislocations is still somewhat clouded in mystery. Several exotic physical phenomena due to these high-velocity dislocations have been proposed but by lack of unambiguous evidence, debate on this topic has been ongoing since its inception in 1949.

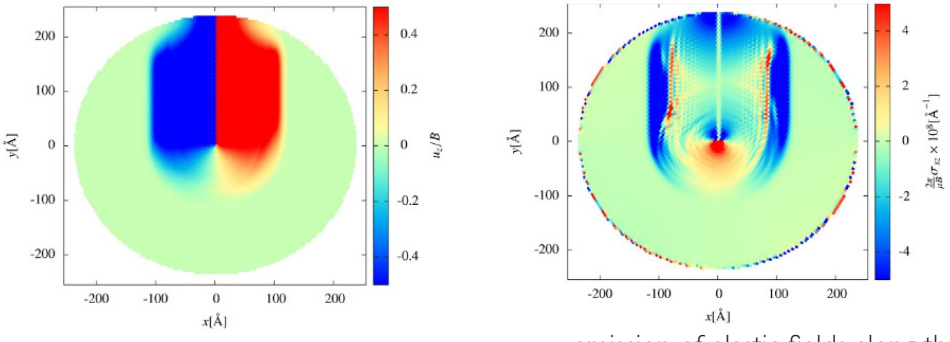


Fig: Elastic fields along the cut plane at the atomistic scale.

Attempts to bring some clarity in this discussion are hampered by the fact that in this regime the usual approximations by which elasticity theory is linearised break down. More recently, increases in computing power have allowed investigations into this problem using atomistic molecular dynamics (MD) and discrete dislocation dynamics (DDD) simulations. In this context, MD is most often used to determine material parameters which are fed into the higher-scale DDD simulations. The most important of these is the relationship between the applied stress and the resulting dislocation velocity: the dislocation mobility. A second ingredient which needs to be introduced into DDD from the atomistic scale is dislocation injection, a way of introducing new dislocations in the material. Previously, B. Gurrutxaga-Lerma showed that for DDD simulations of fast-moving dislocations this should be done in a fully elastodynamic way as opposed to the usual instantaneous elastostatic injection mechanism. This eliminated causality violating dislocations appearing ahead of the shock front and this elastodynamic description was incorporated in D3P, a fully elastodynamic dislocation plasticity code[1].

In this work[2], these elastodynamic dislocation injection fields were simulated on the atomistic scale for screw and edge dislocations. These MD simulations highlighted the existence of an emission of elastic fields along the entire cut-plane (Fig). These are the result of the non-instantaneous character of the injection in the fully elastodynamic picture. They arise as the atoms nearest the cut-plane are necessarily forced through non-lattice positions for a finite amount of time during injection. After the injection, the perfect lattice is restored across the cut-plane but leaves behind an introduced dislocation. These atomistic emission fields were then incorporated in the higher-scale D3P expressions for the injection fields mentioned before. This work was the first step in a wider investigation into the dislocation mobility of fast moving dislocations and in particular which atomistic mechanisms affect it.

1- B Gurrutxaga-Lerma, DS Balint, D Dini, DE Eakins, AP Sutton, Proc. R. Soc. A 469 (2156), 2013

2 - J Verschueren, B Gurrutxaga-Lerma, DS Balint, D Dini, AP Sutton, JMPS 98 (366), 2017

CDT Life
TSM Annual Conference

Sophie Finnigan ***reports on the days events of a successful TSM Annual Conference.***

June saw the TSM-CDT convene for the 4th annual TSM conference. As a rare meeting for the whole CDT, this student organised event saw contributions from all four years. Staff and members of the International Advisory board also attended, allowing for a full celebration of the CDT.

The day was centred around a series of 15 minute talks given by cohort 5, now in the finishing straight of their PhDs, highlighting their research and experiences from the last few years. Cohorts 6 and 7 presented posters, providing engaging discussions to a backdrop of coffee (the academic's staple) and bustling buffet lunch. The newest intake (cohort 8) took to the judging panel, deciding the outcome for both the best oral presentation and poster.

Showcasing the breadth of the CDT, talks and posters covered diverse areas from hydrogen production by polymer photocatalysts (Drew Pearce) to modelling multiscale delayed hydride cracking in nuclear reactors (Mitesh Patel). The prize for best talk was a hotly contested field with Chris Knight and Amanda Diez sharing the win. The winning talks explored their respective research into the simulation of polydisperse granular materials and into the processes of drug delivery

Below: Engaging discussions, drinks and posters. Mid-left: The international advisory board.

by nanoparticles contained in a 'quantum rattle'. Winning the coveted poster prize, with an engaging summary of how cells can be understood by effective potentials, was Ignacio Bordeu (cohort 7).

Alongside these prizes there was a celebration of both the academic and extracurricular endeavours by members of the CDT. Amongst these were several commendations for contribution to life outside the CDT and an unconventional awarding of the Johnson Matthey PhD prize to Michael Ridley (cohort 4) by a Skype call to Tel Aviv where he has begun a postdoctoral position.

Closing the occasion, keynote speaker Prof. Ellen Williams delivered an insightful talk illustrating current materials science initiatives within the energy industry. The talk highlighted the demand and importance for both materials innovation and for the progression of research into tangible prototypes in order to meet the necessary energy targets. Current American policy led to a stimulating field of questions and discussion, reminding me of the larger world within which our fundamental research fits.

Overall, the showcase of research and the recognition of the achievements of the CDT students resulted in a successful celebration of the past 12 months.

Cohort 8 Go Nuclear

Marie Rider ***regales Cohort 8's trip to Culham Centre for Fusion Energy (CCFE).***

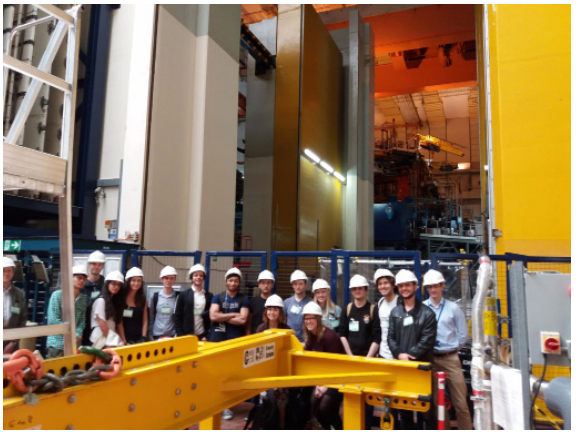
At slightly too early on a Friday morning, cohort 8 gathered outside the Whitely Suite to travel together to CCFE, the UK's forefront centre for fusion energy based just outside of Culham, Oxfordshire. On arrival, we met with our host Prof. Sergei Dudarev who plied us with coffee before we were given an overview of the centre and its various scientific programmes by Martin O'Brien, the centre's director of new research opportunities.

We then ventured to the JET buildings, to see first-hand the control centre, robotics centre and the hangar housing JET, the world's most powerful tokamak.

Next we headed to the newly built Materials Research Facility, where we were given an introduction to the multitude of micro-characterisation methods used at the centre. We peered over the hot cells from the overhead viewing gallery, in which neutron-irradiated material will soon be processed and analysed.

At lunch we were joined by Andrea Sand, who specialises in primary radiation damage in materials, visiting from Helsinki. We spent our remaining time at CCFE with her, Sergei and Max Boeleininger (a TSM student from cohort 4) discussing the multiscale treatment of radiation damage in Tungsten. Exploring various mechanisms that need to be understood in the modelling of interacting defects and dislocations, we brainstormed ideas around the unsolved problems in the theory of high temperature annealing in irradiated materials

Overall, our day at CCFE was scientifically stimulating and illuminated an area of work in which international collaboration is needed from both the academic and industrial communities. With a need for deep understanding of both materials science and physics, the centre showcases a very important platform from which graduates of our CDT can hope to make an impact in their careers after Imperial.



Hard hats for 'proper' engineers as JET peaks through in the background.

Cohort 8 would like to give their thanks to all of the staff and academics at CCFE who made time to engage with us and make the day so memorable. We also extend our thanks to the TSM-CDT staff for organising the trip for us.

Source: https://www.euro-fusion.org/jet/jets-main-features/

Globetrotting

Travelling to worldwide conferences is a definite perk to TSM-CDT life. Here are some of this year's TSM travel tales:

MSc Conference

Sam Palmer looks back on the perfect end to a Masters year with the MSc conference trip heading to EUROMAT in Thessaloniki.

Thessaloniki, Greece, is a city soaked in history, culture, and sun - and coincidentally, also the destination of Cohort 8's chosen conference, EUROMAT 2017. The conference was held in the Thessaloniki Concert Hall, a short, pleasant walk along the sea from our hotel. For many of us this was our first trip to a heavy-weight conference. The program boasted 22 parallel sessions and certainly opened our eyes to the scale of international materials research. The sessions on critical materials were a personal highlight, drawing attention to the need to minimise or replace the use of rare earth magnets in technologies such as electric cars or wind turbines if these technologies are to be mass produced and available to all. Although we were not presenting our own work, the conference was an excellent opportunity to compare many styles of presentation, and I have no doubt that the experience will influence our talks and posters in the future.

White tower views and the conference venue

Answers: b, a, c

Cohort 8 taking in the views from the top of the Concert Hall

Of course, it wasn't all work. We explored the museums and landmarks of the city, which is rich in Byzantine history, and enjoyed Greek food at every opportunity. Luckily, Aliki and Angeliki, the Greek contingency within our cohort, saw us through the large mezze menu ordering experiences safely.

Overall, the week was an incredible learning experience both academically and culturally. A delayed return flight coupled with a city guide book even spawned the 'Test-aloniki!' quiz. Most importantly however, we came out of the experience as a tighter-knit group of friends with lasting memories to look back on.

Test-aloniki!

In what year did the great fire destroy a large part of Thessaloniki?

a. *1901* **b.** *1917* **c.** *1932*

What colour is the waterfront tower, now a museum and monument, named after?

a. *White* **b.** *Black* **c.** *Red*

What was princess Thessalonike of Macedonia's (who the city is named after) relation to Alexander the Great?

a. *Mother* **b.** *Lover* **c.** *Half-sister*

Rob Charlton & Chris Ablitt
APS March meeting - New Orleans, USA

Rob: Experts and students from a great variety of fields come together to share their discoveries, making it hard to decide what to listen to at any given time.

Chris: Although at first a little daunting, it was great to hear about research in my own and other fields as well as checking out the jazz and fried crocodile that the Big Easy is famous for.


Credit: A. Mostofi

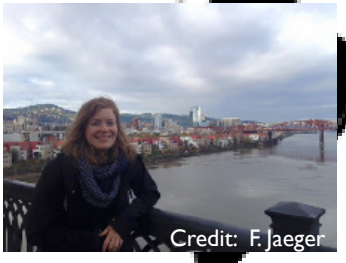
Eduardo Ramos Fernandez
6th World Tribology Conference - Beijing, China

The most important conference in the field with more than 800 presentations (yay!). It was a culturally enriching experience in a city where vestiges of the Communism and iconic symbols of Capitalism blend in a very paradoxical but beautiful way.

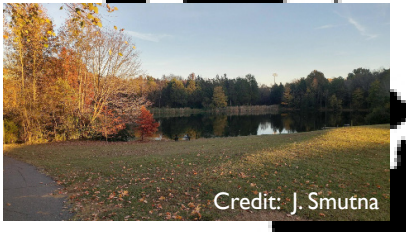
Emanuele Galiffi
London Plasmonics Forum 2017 - London, UK

This gave me a chance to start understanding what research goes on in the field. We visited labs and made jokes about experimentalists! How could a working day be better?


Credit: F. Jaeger


Credit: F. Jaeger


Credit: F. Jaeger


Credit: J. Smutna

Frederike Jaeger
APS DFD meeting - Portland, USA

My yearly trip to the APS DFD was a little more interesting this year as it was right after the US election and we saw some Anti-Trump protests. That didn't detract from the yummy doughnuts, beer and great conference talk titles ('Make water entry great again!').

Jana Smutna
MUZIC Meeting - Charlotte, USA

A great opportunity to hear enthusiastic feedback on the early stages of my work, I also got to visit (and be jealous of) the beautiful University of North Carolina campus.

Sneak Peek
Hermes Summer School 2018

***Nikoletta Prastiti** recalls her Hermes experience and what to expect from Hermes 2018.*

In July 2016, I was given the fantastic opportunity to participate in Hermes 2016. Hermes is an international summer school committed to excellence in materials modelling and science communication. This interdisciplinary summer school is organised solely by PhD students from a variety of institutions and features world renowned academics who deliver engaging talks and a series of innovative workshops and masterclasses to postgraduate students.

The event takes place at Cumberland Lodge, a unique conference centre in the heart of the Windsor Great Park. Its patron, The Queen, has granted sole occupancy of a beautiful 17th-century house for discussions aimed at the betterment of society.

The duration of the summer school was four days. I remember, as if it was yesterday, meeting our roommates and the "ice-breaker" challenge which gave us the opportunity to explore the area while at the same time getting acquainted with the rest of the participants. The next few days included a series of masterclasses in various topics of material science, as well as technical workshops in Mathematica, data visualization and development of presentation skills. We also had the opportunity to boost our teamwork skills by collaborating in mini projects and on the last day demonstrated our acquired skills with a presentation on a self-chosen topic.

Above: 2016's Hermes attendees. Right: Previous summer school presentation

A handful of us, inspired by our experience attending Hermes 2016, decided to lead the organisation of the next Hermes summer school. As we progressed, we were fortunate enough to gain more students interested in helping out. Now, the whole team has come together, each bringing their own ideas and enthusiasm to make this event happen and to ensure that the experience of future participants is just as good as ours was, if not better!

This year's Hermes will feature prestigious academics from various universities including Prof. Daniele Dini (ICL) and Prof. Maria Ramos (University of Porto) amongst others. Moreover, we'll have Baroness Julia King Brown as a keynote speaker to inspire us with her bright career as an academic at Cambridge University and as the head of Materials at Rolls Royce alongside her experiences in the House of Lords. Participants will also have the opportunity to attend talks from scientists who followed alternative career pathways to academia. Particularly, Jassel Madavia a TSM alumna and a founder of Hermes, will share her experiences working as a technical consultant at IBM and now as a data scientist at HSBC. This year's Hermes will also feature industry representatives from Quantumwise to demonstrate their powerful software for modelling materials in the atomistic and molecular scales. Carefully designed workshops will also provide opportunities to develop networking, teamwork and communication skills. We look forward to seeing you at Hermes!

Hermes 2018 will take place 19th-23rd July Applications open in January 2018. Visit http://hermessummerschool.org to find out more.

Camera, Lights, Animation!

Eduardo Ramos Fernandez ***on tackling the silver screen, producing a TSM-CDT promotional video***

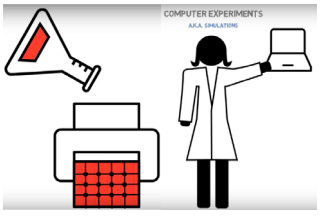
A brand-new exciting TSM-CDT promotional video has been released this year! This is a masterpiece accomplished by several members of Cohort 6.

The aim of the video is to promote the current importance of theoretical and computational research in the field of Materials Science.

The inception of the project dates back to the beginning of 2016's summer. While Hikmat, Lars, Gleb and myself were having an attempt at mexican fajitas at Gleb's place, we realised that we all found it satisfying when we could effectively communicate our research to the non-scientific people close to us. After a not so extensive debate we agreed that a video for the the general public was the way to go. We tried to attract more willing-to-help help Cohort members and in the end Alise and Iacopo decided to joined our group of padawans.

At the time, none of us were skilled in producing any type of multimedia content. It was a real challenge to walk the path of the jedi, but our Yoda guided us through when the project seemed to be falling to the Dark Side. Eventually, the Force awakened and after a few iterations of intense discussion and video editing, we had something to be humbly proud of. It is worth saying that the BBC Communications Course and Hermes Summer School turned out to be fantastic sources of inspiration and resources for us during this project.

Enjoy the video and… May the Force Be With You.



Watch here: https://www.youtube.com/watch?v=BaulD-IjWKvI

Social Round-Up

Festive feelings...

With the Christmas season approaching it was time for the MSc students to remember that there is more to life than learning new things and to organise the annual Christmas party.

Here: Enjoying the festivities and right: Hyde Park football gets compeititive

Utilising the musical vein in the cohort, the evening started with a little music, closing on the notes of Jingle Bells. With plates and glasses definitely half-full, the next thing on the program was an amusing quiz full of science-inclined questions, from the history of science to back-of-the-beer-label calculations. The night ended with a treat as Alise and her choir suddenly appeared to close the night on Christmas carols.

...& Summer Sun

Summer saw the CDT regroup for the annual BBQ and to enjoy their share of the 'summer' weather. To raise appetites (and competitive spirits) a game of football was held first in Hyde Park with some impressive performances.

Taking the post-match analysis up to Blackett level 8, Emanuele 'Grill' Galiffi manned the BBQ and with a team of cohort 8 sous chefs kept burger buns filled. A great evening and an opportunity for all of the cohorts and staff to relax and mix.

Something to Puzzle Over

E	S	C	I	S	Y	H	P	M	K	S	N	C	D	E
C	K	C	Q	U	D	O	S	E	C	W	I	D	I	L
T	V	T	I	C	Q	I	D	H	C	L	K	R	S	A
M	I	F	U	T	T	L	R	T	M	A	Z	I	L	C
P	I	J	V	E	A	O	B	B	A	Q	L	S	O	S
E	Q	B	N	Q	D	M	X	A	L	Q	C	P	C	I
J	O	G	N	I	R	E	E	N	I	G	N	E	A	T
B	A	O	N	V	T	M	L	H	Z	Q	O	V	T	L
M	R	G	R	A	N	E	Z	X	T	U	C	E	I	U
C	E	W	L	B	F	X	L	D	T	A	Q	E	O	M
R	C	H	E	M	I	S	T	R	Y	E	M	R	N	H
S	Z	E	O	J	G	T	E	A	Z	I	B	A	S	V
P	G	W	H	Q	M	A	A	G	K	W	H	N	R	R
E	F	O	O	D	C	Q	S	L	M	H	A	D	B	B
C	I	C	H	H	L	M	Q	H	S	B	V	A	Z	F

1. S, P, D. We are not talking about German politics, but about… (8 letters)
2. In terms of transforms, it is Fourier's little brother, but beware: it is easy to go there, not as easy to come back. (7 letters)
3. The keyword that opens every door in the TSM-CDT. Just abuse it in your presentations. (10 letters)
4. The solution of this equation is the holy grail of all physicists. (11 letters)
5. Some may think these are just a sports injury but here we learn that they are much more. (12 letters)
6. Our beloved administrators for this year... (8 letters)
7. It attracts the opposites. (9 letters)
8. It keeps us all going, and at Imperial it often comes for free. (4 letters)
9. Whether it is over a pint or in a school, it is important to do… (8 letters)
10. It would be a common rubber, if it were not for a chi. (5 letters)
11. Of the four main disciplines we aim at bridging together, the elegant one… (7 letters)
12. ...the fundamental one, (11 letters)
13. ...the reactive one, (9 letters)
14. ...and the dirty one. (11 letters)
15. When it comes to the money, we are all grateful to them. (5 letters)

See the back page for the solution

Outreach
Festival Fever

Outreach officer Simon Foster recalls the success of the TSM stand at this year's Imperial Festival.

The Imperial Festival is an annual science festival which gives the public a chance to go behind the scenes and explore all of the groundbreaking science happening at Imperial College. This year's festival was held over the weekend of the 6th and 7th May, with over 15,000 members of the public visiting Imperial College. Students and staff from the Centre for Doctoral Training in Theory and Simulation of Materials (TSM) hosted a stand in the Discovery Zone discussing how materials research can be taken from the lab and into the real world. Not only does the stand allow us to directly communicate our research to the public, but it also gives postgraduate students and postdoctoral researchers an opportunity to practice and develop their public engagement skills.

The stand was used to publicise the recent opening of the High Performance Computing facility which the TSM group is involved in through our work with the Thomas Young Centre. Using a cluster of 10 Raspberry Pi processors, visitors raced against the computer to solve the Tower of Hanoi puzzle.

Outreach in action: Ignacio Bordeu (Cohort 7) mans the stand

The puzzle consists of 3 rods and 3 discs stacked in ascending order of size on one of the rods. The objective of the puzzle is to move the entire stack to another rod, obeying the following simple rules:

1. Only one disk can be moved at a time.
2. Each move consists of taking the upper disk from one of the stacks and placing it on top of another stack.
3. No disk may be placed on top of a smaller disk.

Lars Blumenthal (Cohort 6) engages the crowd of potential future TSM students

Visitors at first race against only one processor, which they are able to defeat, but as more and more processors are added, the cluster of Raspberry Pi's gets faster and faster until it is able to solve the puzzle quicker than a human. The fastest visitors were placed onto the TSM leader board, with the fastest each hour winning a materials themed prize. Using this demo allowed the public to get hands on with a simple parallel computer set-up, forming the basis of discussion between the public and the visitors to the festival. Monitoring the number of participants showed that more than 500 members of the public interacted with the volunteers on the stand, a triumphant success!

Pints, Pubs and Science

Andrew Warwick, Lara Roman Castellanos and Fangyuan Gu on organsing another successful Pint of Science.

TSM was once again (heavily) involved in the annual 'Pint of Science' festival this year; not only did we help organise events but Chris Ablitt and Rob Charlton (Cohort 6) also coordinated the entire 2017 Pint of Science London series. For their achievements, Chris and Rob won the President's Inspirational Partner Award for Excellence in Societal Engagement.

Starting at Imperial College London, the non-profit festival aims to communicate science of all disciplines to the general public and now takes place in over 175 cities across the world.

The London events covered a wide range of topics in science and technology. Cohort 7's Nuttawut Kongsuwan was involved in the series themed 'Our Society' (taking place in the Australian Embassy, no less!) While our team worked with Benjamin Dive and Zoe Holmes from the Controlled Quantum Dynamics (CQD) CDT under the theme 'Atoms to Galaxies'. Together, we organised 3 nights of talks from 6 speakers.

'Atoms to Galaxies' aimed to provide a perspective of different length and timescales. In one extreme, we invited Professor Arttu Rajantie and Dr. Sarah Malik to give talks on cosmology, from dark matter to the Higgs boson. On our 'Small is beautiful' evening, Professors Vlatko Vedral and Winfried Hensinger showed us the quantum nature of the universe. Moreover, on the final night our own Professor Adrian Sutton and Dr. Johannes Lischner gave a tour on more 'modestly' sized systems.

Above: The Pint of Science team, Left: the stage is set for a night to remember.

Adrian started the night with his aptly titled talk 'Many Mickles make a Muckle'. Using videos of his home-owned bubble raft, Adrian gave the audience an entertaining introduction to dislocations and other types of crystal defects. The parallels drawn between people and a population of defects certainly caught the pub's attention - "some defects seem to have a life of their own, moving at high speeds, multiplying, and working together to create less benign defects".

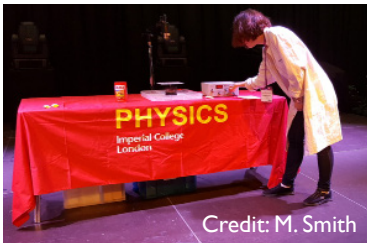
Concluding the night and the Atoms to Galaxies series, was Johannes' 'DIY nanotechnology' session. Amidst his presentation on Graphene, armed with pencils and tape, the audience was invited to make some of their own via the notorious Nobel-prize winning 'scotch tape method'; all done over a pint too.

The 3 nights we hosted were truly memorable and, just as importantly, a lot of fun. It was great to have members of Cohorts 5 through to 8 from TSM and CQD helping out on each night. As far as outreach activities go it's a unique experience to purposely bring science to pub talk and hear so many insightful questions from the public.

Outreach from the Off

Jana Smutna ***tells us about getting involved in outreach from the start and a day making music with the*** *London Philharmonic Orchestra.*

Over the past few years, the list of outreach activities that the TSM-CDT is involved with has been steadily growing. Organising, volunteering or just going to these events is always very rewarding. Not only can you learn about science in a more entertaining way but you also have an opportunity to see your own research in a new light when explaining it to the general public.



Lab coats and all! Demonstrating science with the London Philharmonic Orchestra

During the MSc year, there wasn't the time to get too involved with the organisation of big events. However, there were still many opportunities to get involved just for a day and help out with running an event. "Conducting Science" with the London Philharmonic Orchestra was one such event. There, children had an opportunity to try out some hands-on music by making their own musical instruments and to understand the science behind it. The 'science' volunteers (all dressed in lab coats which most of us haven't worn in years) were showing demonstrations about waves, sound and resonance. It was amazing to see everyone getting so excited about understanding how things work. Getting this response to talking about science from the general public is really motivating and helped me to get through the chaos of the Master's year, while not taking away too much time from the coursework!

A Different Kind of Medication

Eduardo Ramos Fernandez ***on organising the*** *Pain relief for Scientific Computing* ***fair.***

Have you ever experienced frustration using a piece of scientific software? Do you organize, store and process your research data efficiently? Are you taking advantage of the computational facilities/services the College offers you? If the answer is "no" and you are an incipient researcher, you might be interested in attending the Pain Relief for Scientific Computing fair next year.

As part of a group of students from CDTs across the college we organized a one-day fair to infuse new PhD students with good practices and modern approaches in Scientific Computing. There were presentations, posters and stands about a variety of topics such as data structures, version control with Git, High Performance Computing and... tons of pizza!

Stands and talks delivered tips and solutions

It was a very exciting opportunity to mingle with new cohorts of PhD students as well as senior academics who came to the stands to chat about geeky topics like parallel computing and software development. With a turnout of over 60 people it was a real success given that it was the very first edition of the event. The day culminated with a networking session with beers and pizza on hand.

We are aiming to grow bigger and better for next year so stay tuned!

Source: cytora.com

Branching Out

Six Months at Cytora

Chris Knight (Cohort 5) shares his experience entering the world of data analytics, interning with Cytora.

What's the problem with PhD's in the workforce these days? Very bright but no real world experience I was told. What's the solution? Do an internship I was told. It was on this advice, received at the careers planning course in the splendour of Cumberland Lodge, that I, along with many of my cohort 5 peers, decided to undertake an internship at a London based tech company.

There is a growing demand for technically minded people who are able to grapple with the ever growing quantities of data produced by both smart devices and people interacting with technology and digital content more than ever before. There is a thirst for insight from this valuable resource for many worldwide applications, including:

- Increasing the efficiency of industrial processes and business practices, thereby improving profit margins
- Identifying pressure points and improving the provision of government services
- Tackling big problems such as climate change
- The intervention by malicious actors in democratic processes...

... the list goes on.

Having a background in advanced maths, high performance distributed computing and data analysis techniques, as well as the ability to interpret, visualise, understand and communicate complex information to audiences of all levels, TSM students are well positioned to take on these challenges.

During six months away from my PhD, I gained that important real world experience, sharpened my coding skills, learnt about an abundance of new and exciting technologies, and immersed myself in the business mindset and culture. I worked at Cytora, a company co-founded by Aeneas, a TSM cohort 1 alumnus. Initially, the company's focus was on extracting information from a real time stream of around 4 million news articles per day. My first project at the company involved

taking Cytora's data and injecting it into a database in real time, in order to enable analytics which would provide insight for Cytora and their customers. Halfway through my internship, the company's focus changed and in turn my role changed in response. Being exposed to the dynamic nature of a start-up was a great lesson in the way that a successful business' offerings must always be in tune with what the market demands.

Working at Cytora never felt like "work" as I found that each day brought something new and interesting. I made some great friends at the company and expanded my network in a meaningful way. I was able to put the skills gained during my PhD studies into a fresh context and gained new experience which stands me in good stead for my future career. It's for all these reasons that I fully endorse those knowledgeable voices at Cumberland Lodge and recommend an internship to any current TSM students that may be interested.

Credit: A. Diez

An Unusual POST

Amanda Diez (Cohort 5) tells us about her internship at POST, embracing the world of policy making and Quantum Technologies.

Last year, I spent three months at the Parliamentary Office of Science and Technology (POST). POST has eight scientific advisors and approximately eight postgraduate fellows. Fellows are PhD students (and in some cases postdocs), who are assigned a 3-month project under the supervision of one of the advisors. In most cases you are in charge of researching and drafting a POSTnote: a four-page briefing for MPs and Peers published in Parliament's website.

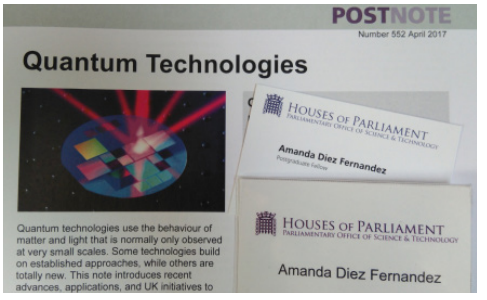
During my first week, I was introduced to my topic: Quantum Technologies, and asked to write a one-page briefing document which I would send to the people I asked for an interview. For the interviews, I then had to suggest a list of stakeholders from academia, industry and the public sector who I would like to talk with.

Set up with a Parliament email account, telephone number and business cards I was encouraged go to the debates in the House of Commons, book tours of the Palace of Westminster, and explore the different Parliament buildings.

Interviewing people was a completely new experience. Some conversations were in person, others on the phone. Some were half an hour long, others more than two. Occasionally I travelled: I went to Birmingham where I saw the facilities of the Quantum Hub, to Oxford, and to Teddington, where I visited the National Physical Laboratory and their atomic clocks.

Learning about Quantum Technologies from top experts in the field was a luxury. My job was a bit like that of a journalist; in fact, at some point, one of the academics I was speaking to said by mistake: "last week, I was telling another journalist"…

The research itself was extremely interesting. Suddenly, I was learning about topics such as cyber security, time stamping to avoid fraud in the financial sector, or using gravity sensors to detect pipes underground. I learned about the worldwide race to produce a quantum computer and the different approaches being taken.



The last interviews occurred simultaneously to the drafting process, which involved careful selection of the content and language due to the strict word limit and the vast subject of Quantum Technologies. It was followed by an exhaustive two-stage review process, in which I had to collate and contrast the comments of more than twenty reviewers.

Work at POST was very different to my PhD in some aspects, while in others it felt very similar. Fellows have a separate office next to the main one, which felt a lot like our own PhD office. Your supervisor has a physics PhD and could have well been your University supervisor. I worked very closely with my supervisor and felt very comfortable and well supported in my project.

I would recommend the experience to everybody, regardless of whether you are interested in science for policy making or not.

Careers

Alise Virbule ***remembers the lessons learnt from the*** *Careers course*.

On a spring morning, cohort 6, headed once more to Cumberland Lodge, intrigued to find out what the careers course was all about.

Initially, we heard from a panel of successful PhD holders, who work in academic or industrial research, data science and sales. Happily answering all of our questions, they largely confirmed the impressions we had of potential future professions. But a recurring topic, both during and after the course, was networking. On entry, our view on networking was mainly of people selfishly trying to use each other to climb the career ladder. Our panellists gave us a new perspective, although you gain a lot by reaching out to contacts who are further along in their careers, you also give back a lot by helping people who later reach out to you. Additionally, the more you show true interest in people whose work you admire, the more likely you are to find out about work opportunities that would be perfectly suited to you.

Authentity

With the return of *Piero Vitelli's Authentity* ***course,*** *Nuttawut Kongsuwan* ***recounts his experience.***

I started my PhD with the impression that success in science was only determined by an individual's ability and talent. My life at Imperial College could not prove me more wrong, teaching me that successful scientists are those who also excel in teams. Fortunately, my understanding and teamwork ability were greatly reinforced by attending Authentity 2017, a transferable skills workshop which teaches communication, teamworking and networking through engaging activities.

Cohort 7, together with CDTs from Bristol, Manchester and Sheffield, participated in this three-day course at Cumberland Lodge. Starting with presentation techniques and networking tips, we were then separated into random groups and participated in several team building activities. Each activity represented a different aspect of teamwork and gave us understanding of how a team is seen from leaders and followers' perspectives. On the last day, each team incorporated all the newly developed skills into a video which tackled a challenge in our modern society.

Beforehand, we had mainly been excited to find out more about our potential career options than spending time with HR experts discussing how to improve our communication skills. We couldn't have been more wrong. The invaluable feedback we received on our sample CVs, cover letters and answering example interview questions showed us just how little we knew about nailing job interviews. Yes, we'll have our grades and publications to get us into an interview, but there is still a long way to go.

All in all, it was unanimously agreed that it was a great and highly valuable course. I even made a contact that helped me to get an internship at Cytora, a data science startup, which 2 months in I'm enjoying immensely!

Top: The stunning Cumberland lodge.
Bottom: Activities and discussion at Authentity.

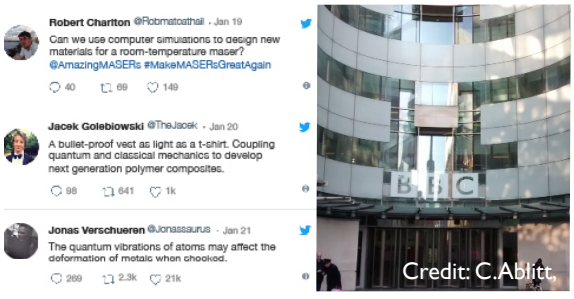
Of course, communication, teamwork and networking skills can not be mastered in simply three days. However, the workshop made us aware of the importance of these skills in our PhD and beyond and led us to take the first step to bring out our inner potential.

Science Communication

Chris Ablitt recalls taking to the airways while attending the Science Communication Course.

3… 2… 1… ON AIR! "Good morning Britain, today I'm joined in the studio by a PhD student from Imperial College London who's going to tell us all about the clever research they've been doing for the last three years…"

This may sound like a dream – or a nightmare – but in January it was a (simulated) reality for Cohort 6 who took part in the 2017 Science Communication Workshop. On home turf in the South Kensington campus, the TSM students were joined by CDTs from Bristol, Sheffield and Manchester for the three-day course examining all forms of Science journalism: TV, radio, print and digital.



Above: Jonas, Jacek and Rob utilising the power of twitter to communicate research. and the BBC studios. Right: A unique classroom for the day

Separated into groups with a mix of students from each CDT, we rotated through a program of sessions studying different media. This was not to be three days spent stuck in a classroom though: within a few hours we had been cast as cameramen, producers, reporters and scientists and were filming our own TV and radio news reports on the Zika outbreak in Central America. Although the amateur dramatics requirement took a few people by surprise, thanks to the expert guidance from Gareth Mitchell and Robert Sternberg, lecturers from Imperial College's Science Communication and Science Media Production MSc courses, we soon came to appreciate the amount of footage and clever editing tricks which go into just a few minutes of news reel.

While one half of the group were starting to fancy themselves as the next Steven Spielberg, the remaining students were taking a masterclass in the fast-paced world of written journalism by Jon Copley, a journalist and co-founder of SciConnect. Jon taught us the tricks to writing a killer press release, but also warned us of the perils of woolly press releases, especially if they get picked up by lazy journalists... This was drummed home in a fun exercise where we selected and wrote headlines for press releases acting as different media outlets (including one unnamed tabloid notorious for click-bait science headlines). It was worrying how close some of our satirical answers came to the truth!

The highlight of the course was, without question, the final morning when we got to visit the BBC studios near Oxford Circus to record our own 20-minute radio broadcasts. With two students taking the helm as presenters, most teams chose to give short interviews with the other guests on their research. One team broke the mould however with a discussion format debating on the trials and tribulations of being a PhD student.

As well as being a lot of fun the course was a useful exercise in learning how to condense our research down to a short description that a non-Scientist might find interesting – something we all have to do! It was also thought-provoking to learn how science journalism works behind the scenes and surely made us all a little more cynical of science headlines!

Onwards and Upwards
Into the Unknown

The level of commitment required for a PhD is unquestionable, so what happens when the years finally come to an end? We caught up with finishing students Peter Fox and Nicola Molinari (Cohort 5) to find out about their plans for the future.

What are your plans for the future now that your time in the CDT is coming to an end and how have these changed since you started?

NM: Many PhDs just roll into a postdoc but I knew that I didn't want to stay in academia. When I first joined the CDT I wanted to go into banking and finance but I've done a lot of research throughout my PhD. I eventually found out that finance jobs sounded boring, so then I thought about management consulting, that was the next one and it sounded amazing.

However, then I did my internship at Bosch in Boston and I experienced doing research in a different context. It was industrial but very fundamental (even using Quantum MC) and it was basically a postdoc, in the sense that it was all your own ideas but reporting to a principal investigator. I realised two things: 1. I was not completely done with research and 2. That I really liked Boston. So I came back thinking of doing a postdoc in Boston. However, I didn't want to do one just for the sake of doing one, I wanted a good one so I looked at Harvard and MIT. After attending APS in America I stopped in Boston and met some professors at MIT. Then, the guy I worked for at Bosch, Dr. Boris Kozinsky, became an associate professor at Harvard and asked if I'd like to do a postdoc.

...and past the postdoc?

NM: Staying out there, in the US, is the plan. I see myself as more of a manager than a hard science person, so maybe a group manager in industry which does actual research or even higher, potentially something in policy too.

Do you not see the role of a supervisor as a more management role?

NM: I like impact, which is why I like management consulting, and having that impact is easier in politics or industry. In academia you have to compromise in that the number one priority is getting funding, but I am not ruling it out!

PF: I'd like to work in some form of science communication, either as a freelance science writer or broadcaster. Or this might entail a role as an outreach officer or a science communication officer for a charity. Basically, a role which involves taking difficult scientific concepts and relaying it to a lay audience. Working as an editor or associate editor for one of the science publications is another possibility depending on the roles available, so potentially still working in science but not doing science.

Communicating to the general public or to a scientific audience is quite different though, is there not one you prefer?

PF: I guess you don't know if you don't try. I have experience doing outreach and school teaching but I'm also open to trying something more specialist.

NM: I remember that in your spare time you play guitar and make music, have you considered merging music and this?

PF: As Nicola says I write my own songs, play piano and I've done some gigs around London. I did write one science based song, 'Geek Like Me', but would I want to just write songs about science? Probably not exclusively, but maybe I would like to include songs about science in my musical repertoire.

Were your plans always to go into science communication?

PF: I started the CDT with the idea that I may stay in academia, although I was open to other options but I wasn't sure what these would be.

We were told at the start that these options would become clear as we went through and the CDT does give every opportunity to explore careers outside of academia.

NM: What Peter says is definitely true, but I wouldn't entirely rely on the CDT. It gives you the seed to find interest in something else but it's up to you, like Peter did, to pursue that. The CDT definitely helped me, especially the cohort environment.

PF: Nicola is right in that while the onus is on you to go out and do it the cohort means that you have a network there almost automatically.

What motivated you to choose your direction?

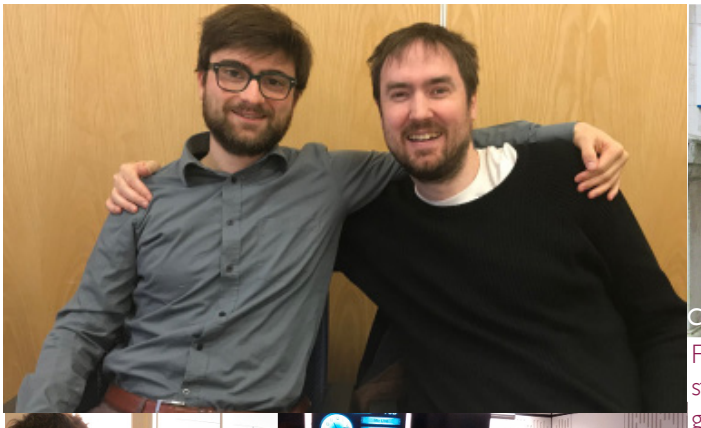
NM: It was mainly the internship at Bosch in Boston. Also the fact that the postdoc is in a completely different field. In terms of motivation, this means that there is this challenge component as it is something I know nothing about.

PF: My main motivator was when we did the Science Communication course, we spent a day at the BBC with Gareth Mitchell who runs the MSc science communications course at Imperial and who also works as presenter on 'Click' on BBC World Service. We all had a go at presenting a show and afterwards others came back saying that I looked really natural, but it was the first time I'd done it. This gave me confidence and I started to write a few articles for iScience (an Imperial general science magazine) and I received good feedback from the editors. The broadcasting led to the writing, this plus the previous experience I have from teaching and doing outreach is the motivation.

What piece of advice would you give each other for their respective pathway?

NM: I really like Peter's attitude to life in general, going from teaching to a PhD to a new direction. I think he's exploring everything he likes and has a very successful life both professionally as an academic and personally, there isn't much advice I can give him!

PF: In response, I think that you're going about it in the right way in not being afraid to change direction, right from the start of your PhD. Keep that up throughout your life, I don't think anyone nowadays thinks that they have a job for life. Keep moving jobs and locations especially while you're young and unattached, which it seems like you're going to do. If you ever do settle back down in London, then contact me and we can go for a beer!



Credit: M. Smith


Credit: M. Smith


Credit: A. Verbule

From above anti-clockwise: Cohort 5 just starting out; Peter and Nicola today; Nicola graduating from the MSc year; the BBC studio from the Science Communication course which inspired Peter's direction and below: Boston skyline, Nicola's next destination.


Source: Wiki Commons

Start-Up Spotlight

Meet the CDT alumni taking different directions.

FIELDING DSP

Fabian Renn, Cohort 2 alumnus, fills us in on his start-up.

Tell us about Fielding DSP.

Fielding DSP writes software which is typically used in the mastering stage of music production. Our most popular product Reviver is now used by hundreds of music producers around the world. However, to put things into perspective, Fielding DSP has always been more of a hobby - we don't have any employees, our turnover is relatively small and all the founders have full-time "real" jobs.

Are you satisfied with what you've accomplished so far?

I have very mixed feelings about how satisfied I am with what we have accomplished so far. On one hand, most of Fielding DSP was really just a giant stroke of luck. We never intended it to be an actual serious company, so in that sense I am super lucky and excited that people are actually buying our product. On the other hand, it showed me that this company could be so much more, if we just invested some more time in it - and this makes me feel unsatisfied. In fact, I was so unsatisfied with this, that I have recently decided to take a two month sabbatical from my "real" work to focus a bit on Fielding DSP. So let's see how that goes...

Can scientific training make for a better entrepreneur?

Yes, I think it does. It's important to have an analytical mind to understand your numbers. It's good to be able to quickly graph, aggregate and analyse certain business results. All skills that TSM-CDT students will be very familiar with.

Sonodot

Recently selected for a start-up accelerator programme, Cohort 2 alumnus Niccolò Corsini gives us the lowdown on Sonodot.

What is Sonodot and how did the idea come about?

During my PhD, a colleague and I won a trip to the GooglePlex in Mountain View through entering a CDT organised business plan competition. The idea was real-time monitoring of crowd dynamics with a low-cost acoustic tracking system and applying chemistry concepts to analyse the crowd's collective behaviour (i.e. treating pedestrians as atoms). By serendipity, one of the leading experts in crowd dynamics modelling was at the conference and got excited about our concept making us realise that there may be more to our little demo than anticipated. Fast forward a few years and here I am working full-time with 3 others on Sonodot. The idea has morphed since and we now focus on helping warehouses and factories increase the efficiency and safety of their material handling operations by tracking their mobile assets.

Can scientific training make for a better entrepreneur?

Definitely. A lot of the qualities that make a good scientist are fundamental to entrepreneurial success. A start-up can be seen as a set of assumptions that require empirical validation through continuous testing. Such tests (e.g. new product features or customer interviews) require methodical design, interpretation and clear communication of the results. On the technical side, I was positively surprised by how transferable a lot of the simulation methods are to our specific problem. The tenacity and patience in the face of uncertainty that are required from an academic are the most crucial component.

What's been the biggest challenge?

The biggest, and ongoing, challenge is building a product people are ready to pay for and surviving with limited resources.

REROO

We found out more ReRoo, an app approaching the market soon, from Thomas Edwards, cohort 3 alumnus and full-time software engineer

What is ReRoo and how was it conceived?

It all started back in April 2015 during Hacktrain, Europe's first hackathon on a train, when my team came up with the idea of a Skyscanner for trains. Essentially, this means combining multiple tickets/alternative routes together for cheaper journeys overall. We decided to call our app ReRoo, because of the re-routing. Our team won the Hacktrain and so we decided to take it forward and found our startup.

After straining to figure out how to develop a robust routing algorithm, we came across a couple of developers who had already solved the problem of network optimisation with regards to split-ticketing. All we needed to do was to process the data from their API and provide a nice shiny user interface!

How did your TSM-CDT background help you?

It helped me in two ways:

1. Programming wise, I gained the necessary precursor skills and I was also surrounded by Python programmers which helped.

2. The atmosphere, the peer pressure from entrepreneurial and hard-working students around me definitely left a mark.

My training has also helped me inject a bit of rational thought into the process of forming a start-up and app development.

Why did you decide to take the leap from scientist to entrepreneur?

During my PhD, I started to consider myself better at software engineering than at scientific research. I was desperate to make a positive contribution to society, so hackathons about climate change and social enterprises became my thing. The skills I developed backend programming for ReRoo helped me get my current job.

Kopernio

From passing his PhD viva in Spring, cohort 3 alumnus Ben Kaube is going from strength to strength with new initiative Kopernio

Tell us about your newest endeavour.

Kopernio is a free browser plugin to help researchers get convenient access to research articles wherever they are. Behind the scenes, Kopernio sources journal paper PDFs and delivers them at the click of a button. While still in beta, Kopernio is used at over 350 universities around the world!

Where did the inspiration come from?

Writing up my thesis I found myself with dozens of browser tabs open trying to lookup references and find journal article PDFs. Compared to Spotify where I could play any song with a single click, the process felt impractical and antiquated. I started to think about solutions and allowed myself the occasional break from writing up to work on a prototype for 'one-click' access to research articles.

Install Kopernio at https://kopernio.com

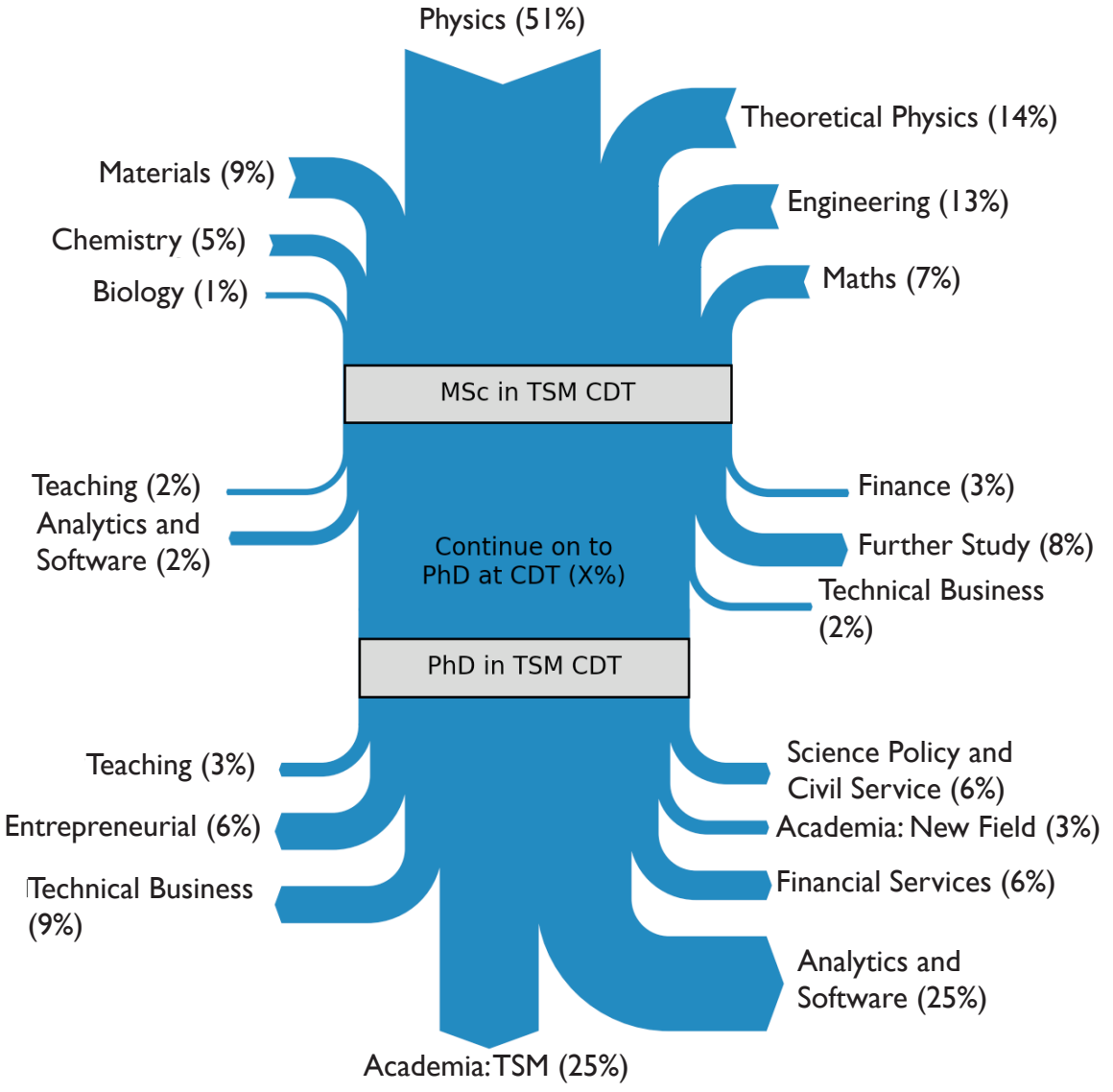
Can scientific training make for a better entrepreneur?

Two important elements of successful entrepreneurship are finding a real problem to work on and having the necessary chops to have a chance at solving it. With scientific training you get exposed to some of the most pressing and interesting problems facing society (sustainable energy, healthcare etc.). Moreover, those with scientific training are in the privileged position of having the skills needed to chip away at these problems and make meaningful progress. In particular, TSM's multi-disciplinary approach fosters breadth of thought which I've found tremendously useful.

Any words of wisdom for current students?

Your PhD is a great time to get involved with entrepreneurial activity. There's support and expertise available around campus so give it a try!

Origins and Destinations



Selected Destinations:

Dr Jassel Majevadia *(Cohort 1)*
Data Scientist
HSBC

Dr Anthony Lim *(Cohort 2)*
Research Fellow
UCL

Dr Valérie Vaissier *(Cohort 2)*
Post Doctoral Scholar
Univeristy of California, Berkeley

Dr Musab Khawaja *(Cohort 3)*
Application Engineer
MathWorks

Dr Daniel Rathbone *(Cohort 3)*
Research Analyst
House of Commons

Dr Christopher Rochester *(Cohort 3)*
Quantitative Analyst
PrismFP

Selected Publications

Discrete Dislocation Plasticity Modeling of Hydrides in Zirconium under Thermal Cycling - M. Patel, S. Waheed, M. Wenman, A.P.Sutton, D.Balint, Discrete Dislocation Plasticity, MRS Advances, 2(55), 3353-3358, 2017

Compacted Dimensions and Singular Plasmonic surfaces - J.B.Pendry, P.A.Huidobro, Y. Luo, E. Galiffi, Science, 358 (6365), 915-17, 2017**S**

Suppressed Quenching and Strong-Coupling of Purcell-Enhanced Single-Molecule Emission in Plasmonic Nanocavities - N. Kongsuwan, et al., ACS Photonics, Article ASAP

The Origin of Uniaxial Negative Thermal Expansion in Layered Perovskites - C. Ablitt, S. Craddock, M. S. Senn, A. A. Mostofi and N. C.Bristowe, Nature Computational Materials 3, 44, 2017

Emergent Properties of an Organic Semiconductor Driven by its Molecular Chirality - Y. Yang, B. Rice et al., ACS Nano 2017, 11, 8329−8338, 2017

Impact of Aggregation on the Photochemistry of Fullerene Films: Correlating Stability to Triplet Exciton Kinetics - E.M. Speller, J.D. McGettrick, B. Rice et al., ACS Appl. Mater. Interfaces, 9, 22739−22747, 2017

The Role of Molybdenum in Suppressing Cold Dwell Fatigue in Titanium Alloys - Adam J. Ready, Peter D. Haynes, Blazej Grabowski, David Rugg, Adrian P. Sutton, PR. Soc. A, 473 (2203), 2017

Topological Photonics: from Crystals to Particles - G. Siroki, P. A. Huidobro, V. Giannini, PRB(R) 96, 041408, 2017

Protection of Surface States in Topological Nanoparticles - G. Siroki, P. D. Haynes, D. K. K. Lee, V. Giannini, PRMaterials 1, 024201, 2017

Non-local model for Diffusion-mediated Dislocation Climb and Cavity Growth - I. Rovelli, S. L. Dudarev, A. P. Sutton, J Mech Phys Solids, 103, 121-141, 2017

The Injection of a Screw Dislocation into a Crystal: Atomistics vs Continuum Elastodynamics - J. Verschueren, B. Gurrutxaga-Lerma, D.S. Balint, D. Dini, A.P. Sutton, J. Mech. Phys. Solids 98, 366–389, 2017

The Influence of Surface Roughness and Adhesion on Particle Rolling - R. Wilson, D. Dini, B. van Wachem, Powder Technology 312, 321-333, 2017

Partition-free Theory of Time-dependent Current Correlations in Nanojunctions in Response to an Arbitrary Time-dependent Bias - M. Ridley, A. MacKinnon, L. Kantorovich, Physical Review B 95, 165440, 2017

Stacking Faults and the Gamma-surface on First-order Pyramidal Planes in Alpha-Ti – A. J. Ready, P. D. Haynes, D. Rugg, and A. P. Sutton, Philosophical Magazine Part A: Materials Science, 2017

Unravelling the Roles of Size, Ligands, and Pressure in the Piezochromic Properties of CdS Nanocrystals - Niccolò R. C. Corsini, Nicholas D. M. Hine, Peter D. Haynes, and Carla Molteni, Nano Lett., 17 (2), 1042−1048, 2017

Electrotunable Lubricity with Ionic Liquids: the Influence of Nanoscale Roughness -Faraday Discussions, A. David, O.Y. Fajardo, A. A. Kornyshev, M. Urbakh, and F. Bresme, 10.1039/C6FD00244G, 2017

Molecular Simulation of Gas Solubility in Nitrile Butadiene Rubber - M. Khawaja, A. P. Sutton, and A. A. Mostofi, Journal of Physical Chemistry B, 121 (1), 2016

Full list: http://www.imperial.ac.uk/theory-and-simulation-of-materials/research/student-publications/

Current Students and Research

Cohort V

Amanda Diez

Structures and Processes in a Quantum Rattle

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

Peter Fox

Nanoplasmonics and Metamaterials at the Classical/Quantum Boundary

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

Frederike Jaeger

Flow of Fluids Though Porous Media with Application to Membranes: from the Molecular to the Continuum Scale

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

Chris Knight

Multi-Scale Analysis of Liquefaction Phenomena in Soil

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

Andrew McMahon

The Behaviour of Charged Species in Hybrid Organic-Inorganic Perovskite Photovoltaics

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

Nicola Molinari

Towards a Predictive Model of Elastomer Materials (with funding from Baker Hughes)

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

Vadim Nemytov

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

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

Premyuda Ontawong

Atomistic-to-Continuum Theory of Martensitic Transformations

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

Farnaz Ostovari

Modelling Damage in Environmental Barrier Coatings on Woven SiC/SiC Composite Substrates

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

Mitesh Patel

Multiscale Modelling of Delayed Hydride Cracking (with funding from Rolls-Royce)

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

Drew Pearce

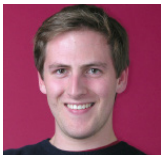
Approaches and Challenges in the Coarse-Graining of Conjugated Molecular Materials

Prof. Jenny Nelson (Physics)

Beth Rice

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

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



Markus Tautschnig

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

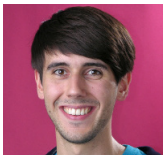
Prof. Nicholas M. Harrison (Chemistry), Prof. Mike Finnis (Materials/Physics)

Cohort VI

Chris Ablitt

First Principles Lattice Dynamical Study of Ferroelectric and Negative Thermal Expansive Ruddlesden-Popper Oxides

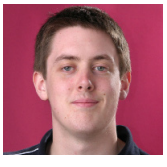
Dr Arash Mostofi (Materials/Physics), Dr Nicholas Bristowe (Kent), Dr Mark Senn (Warwick - Chemistry)



Lars Blumenthal

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

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



Robert Charlton

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

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

Luca Cimbaro

Embrittlement of Ni-based Superalloys by Oxygen (with funding from Rolls-Royce)

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

Jacek Golebiowski

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

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

Hikmatyar Hasan

Designing Next Generation High-Temperature Co-Al-W Based Superalloys

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

Eduardo Ramos Fernández

Multi-Scale Modelling of Hydrodynamic Lubrication and Friction (with funding from BP)

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

Iacopo Rovelli

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

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

Gleb Siroki

Optical Properties of Topological Insulator Nanoparticles

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

Jonas Verschueren

Fundamentals of Dislocations in Motion

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

Alise Virbule

Design of High Absorption Organic Semiconductors for Applications to Solar Cells and Light Emission

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

Marise Westbroek

Flow in Porous Media (with Janet Watson scholarship)

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

Cohort VII

Fangyuan Gu

Controlling structural change in multiferroic materials by ultrafast laser excitation

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

Nikoletta Prastiti

Modelling methodologies for microstructure-sensitive crack growth in aero-engine PM Ni alloys

Dr Daniel Balint (Mech. Eng), Prof. Fionn Dunne (Materials)

Lara Román Castellanos

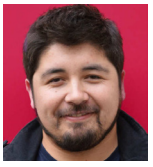
Hot electrons in nanoplasmonics: combining quantum mechanics with nanophotonics

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

Ignacio Bordeu

Theory of active matter (with funding from Conicyt)

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



Harry Cárdenas

Molecular thermodynamic models for adsorption (with funding from Conicyt)

Prof Erich A. Müller (Chem. Eng.)

Mariana Hildebrand

Towards the manipulation of defects and dopants to functionalise graphene

Prof. Nicholas M. Harrison (Chemistry)

Nuttawut Kongsuwan

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

Prof. Ortwin Hess (Physics)

Charles Penny

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

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

Christopher Sewell

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

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

Panagiotis Simatos

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

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

Andrew Warwick

Emergent Phenomena at domain walls in halide perovskites

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

Cohort VIII

Martik Aghajanian

Adsorbate engineering in two-dimensional semiconductors

Dr Arash Mostofi (Materials/Physics), Dr Johannes Lischner (Materials/Physics)

Cristian Constante Amores

Multi-phase modelling of oil-water droplet size districutions (with funding from BP)

Prof. Omar Matar (Chemical Engineering)

Sophie Finnigan

Modelling the decomposition of chemical warfare agents in the environment

Dr Kim Jelfs (Chemistry), Dr Patricia Hunt (Chemistry)

Emanuele Galiffi

Transformation optics applied to plasmons in graphene

Prof. Sir John Pendry (Physics), Dr Paloma Arroyo Huidobro (Physics), Prof. Norbert Klein (Materials)

Syed Hussain

Group theoretic methods for semi-empirical electronic structure of topological materials

Prof. Dmitri Vvedensky (Physics), Prof. Jing Zhang (Physics), Dr Paul Tangney (Physics/Materials)

Samuel Palmer

Simulation of phoxonic metamaterials

Dr Vincenzo Giannini (Physics), Prof. Richard Craster (Mathematics)

Luca Reali

Cyclic loading and delayed hydride cracking in Zr-alloys (with funding from Rolls-Royce)

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

Marie Rider

Quantum optics with topological insulator nanoparticles

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

Jana Smutna

Understanding the role of hydrogen-dislocation interactions in the corrosion and hydrogen uptake of irradiated zirconium fuel cladding alloys (with funding from Rolls-Royce)

Dr Mark Wenman (Materials), Dr Andrew Horsefield (Materials), Prof. Adrian Sutton (Materials)

Anthony Spice

Optical resonances of high-index dielectric nanostructures: Scalings and multiscale asymptotics

Dr Ory Schnitzer (Mathematics), Prof. Stefan Maier (Physics)

Aliki-Marina Tsopelakou

Reaction mechanisms for materials systems with complex potential energy surfaces (with funding from Toyota)

Prof. Peter Lindstedt (Mech. Eng.), Prof. Daniele Dini (Mech. Eng.)

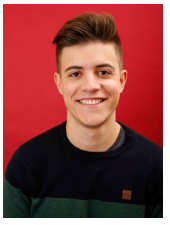
Tomos Wells

Spin-lattice coupling in magnetic materials (with funding from Culham Centre for Fusion Energy)

Dr Andrew Horsefield (Materials), Prof. Matthew Foulkes (Physics), Prof. Sergei Dudarev (EURATOM, Physics)

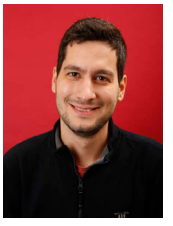
Welcome to Cohort IX!

Zainab Alaithan *(with funding from Aramco)*

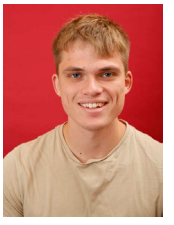


Carlos Ayestaran Latorre *(with funding from Afton Chemicals)*

Alessio Bevilacqua *(with funding from the Materials Department)*

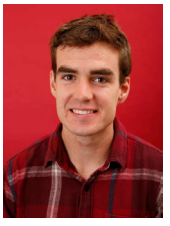


Dimitrios Bikos *(with funding from Nestle)*

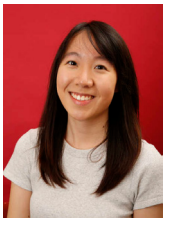


Andrew Borrill

Gabriele Coiana

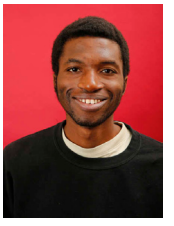


Zachary Goodwin

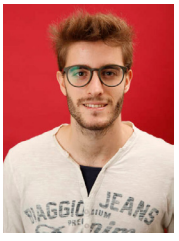


Danielle Ho En Huei

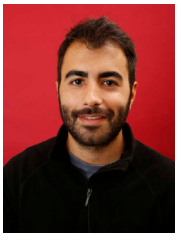
Martin Lazo



Matthew Okenyi

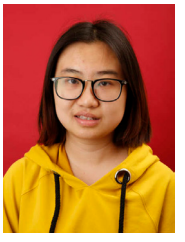


Carles Rafols i Belles *(with funding from BP)*



Georgios Samaras *(with funding from an IC President's Scholarship)*

Rosemary Teague



Yiyuan Want *(with funding from ABB)*

Members of the Advisory Board

External Advisors

Dr Anna Angus-Smyth – EPSRC Representative
Prof W Craig-Carter – Massachusetts Institute of Technology, USA
Dr David Curry – Baker Hughes, UK
Dr Dirk Dijkstra - Covestro Deutschland AG, DE
Prof. Sergei Dudarev – EURATOM Fusion, UK
Dr Claire Hinchliffe – Sheffield-Manchester CDT in Advanced Metallic Systems, UK
Prof. David Rugg – Rolls-Royce, UK
Dr Simon Schultz - CDT in Neurotechnology, ICL, UK
Prof. Helena Van Swygenhoeven – Paul-Scherrer Institute & EPFL, CH
Dr Erich Wimmer – Materials Design Inc., USA/FR
Prof. Ellen Williams - University of Maryland, USA
Dr Hugh Stitt - Johnson-Matthey, UK

TSM-CDT Staff

Dr Arash Mostofi – Director and Cohort IV Mentor
Dr Johannes Lischner – Assistant Director
Prof. Peter Haynes - Strategic Advisory Team
Prof. Adrian Sutton - Strategic Advisory Team
Prof. Mike Bearpark – Cohort Mentor: Cohort VI
Dr Andrew Horsfield – Cohort Mentor: Cohort VII
Dr Kim Jelfs - Cohort Mentor: Cohort VIII
Prof. Daniele Dini - Cohort Mentor: Cohort IX
Dr Simon Foster – Outreach Officer
Ms Miranda Smith – Senior CDT Administrator

For a full list of staff see:
http://www.imperial.ac.uk/theory-and-simulation-of-materials/people/staff/

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Email: miranda.smith@imperial.ac.uk
Web: www.tsmcdt.org

Student Awards

2016 Awards

Major Contribution to the Life of the CDT:
Drew Pearce (Cohort 5), Chris Ablitt, Iacopo Rovelli, Rob Charlton, Jacek Golebiowski, Jonas Verschueren (Cohort 6)

Outreach Prize :
Beth Rice (Cohort 5)

Julian Walsh Prize for the Outstanding Contribution to the Life of the CDT:
Lars Blumenthal (Cohort 6)

Material's Design Advanced Graduate Research Prize:
Mitesh Patel (Cohort 5)

Material's Design Early Stage Graduate Research Prize:
Chris Ablitt, Gleb Siroki (Cohort 6)

2017 Awards

Johnson Matthey PhD prize:
Michael Ridley (Cohort 4)

Sutton Prize for the Best Overall Performance in the TSM MSc:
Martik Aghajanian (Cohort 8)

Some of the above prize winners.
Top (Left-right): Chris Ablitt winner of the Material's Design Early Stage Graduate Research Prize; Drew Pearce and then Chris Ablitt and Iacopo Rovelli, all recipients of the Major Contribution to the Life of the CDT prize.
Bottom: Ignacio Bordeau, Amanda Diez and Chris Knight, prize winners at the TSM Annual Conference 2017

Word Search Solution

Solutions:

Orbitals, Laplace, Multiscale, Schrodinger, Dislocations, Veeranda, Magnetism, Food, Outreach, LaTeX, Physics, Mathematics, Chemistry, Engineering, EPSRC.

Made by Luca Reali using puzzlemaker at discoveryeducation.com

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+ S C I S Y H P M + S + + D E
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+ A O N + T + + H + + O V T L
M + G R A + + + + T U + E I U
C E + L B + + + + T A + E O M
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P + + + + + A A + + + + N + +
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(Over,Down,Direction)
  CHEMISTRY(2,11,E)
 DISLOCATIONS(14,1,S)
 ENGINEERING(13,7,W)
   EPSRC(1,14,N)
   FOOD(2,14,E)
  LAPLACE(15,8,NW)
   LATEX(4,10,NE)
 MAGNETISM(1,9,NE)
MATHEMATICS(12,11,NW)
 MULTISCALE(15,10,N)
  ORBITALS(3,8,SE)
 OUTREACH(12,8,SW)
  PHYSICS(8,1,W)
SCHRODINGER(11,1,SW)
 VEERANDA(13,8,S)
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Editor's Backword

We hope that you've enjoyed this year's Annual Report. We would like to make a special thanks to Miranda Smith for all of her help during the editorial process and for having the answer to every question that we asked!

Back cover: Sophie Finnigan

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