Annual Report

2014-2015

Centre for Doctoral Training in Theory and Simulation of Materials

"Scholarship that is indifferent to human suffering is immoral"

—Richard Levins, Living the 11th Thesis, 2008

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London, November 2015

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Director's Foreword

SIX YEARS on from opening our doors to our first cohort of students, we have now seen a sufficient number of graduates to be able to reflect on the value added by the Centre approach to doctoral training. In the first edition of this annual report published in 2012, I explained the multidisciplinary mission of the TSM-CDT 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 time scales. The requirement to involve two supervisors with complementary expertise at adjacent scales generated a new network of inter-departmental collaborations across Imperial College and beyond and ensured that CDT projects were not simply "more of the same" that were already funded by other mechanisms.

But our mission statement encapsulates a more fundamental distinction between the Centre and "traditional" approaches. In the latter case, normally a single supervisor works with a student and the focus is on the project – with outputs typically measured in terms of publications and invitations to speak. That relationship still exists within the Centre model, and is vital to ensure the scientific excellence of the research carried out. But the Centre adds a second focus on the person rather than the project. The "outputs" of a CDT are principally the people that it produces. As a result, most of the work of the TSM-CDT aims to enrich the student experience through cohort-building activities, mentoring, bespoke professional skills training, career planning, networking and outreach. Moreover, the ethos of student leadership pervades all of these activities: rather than seeking to fill up the diaries of our students, we provide them with the opportunities and resources to organise events that they are enthusiastic about. As ever, this report is written by the students about the activities that they have chosen to be involved with, and I am delighted to see that the array is as impressive as ever.

By far the most enjoyable aspect of my time as Director of the TSM-CDT has been interacting with the talented students who have joined us. I took up a new role as Head of the Department of Materials in July, and during the coming year I will be standing down from the TSM-CDT and handing the directorship over to the very capable hands of Dr Arash Mostofi, the current Assistant Director. I am sure that he will find it to be just as rewarding a job as I have.

Peter Haynes

Contents


Source: L. Blumenthal

Cohort 6 : On the Way to Lille

Lars Blumenthal *and* ***Hikmatyar Hasan*** *recall Cohort 6's trip to E-MRS in Lille.*

Every year the TSM-CDT's newest cohort is taken to an international materials related conference. Previous cohorts travelled to the farthest corners of the world, such as Singapore and San Francisco. This year, however, sensible thinking prevailed, and the members of cohort 6 were ushered to Lille, France for the European Materials Research Society (E-MRS) Spring Meeting. We were told of all the perks, such as no jet lag and Belgian beer and the trip did turn out to be a great success.

Source: L. Blumenthal

After traveling with the Eurostar underneath the English Channel, we had enough time to enjoy a steakhouse dinner and settle in our rooms, ready for a busy time of 'conferencing' the next day. Although the conference was mainly for experimentalists, we managed to blend in and everyone was free to see the talks they were most interested in. Soon, it was apparent to everyone that just listening to all the different speakers was more tiring than first expected. This was not because their talks were boring but because one can only absorb a certain amount of information each day. However, the organisers of the E-MRS Spring Meeting allowed for enough coffee breaks to block our adenosine receptors and provided a three-course lunch to fuel us too. For dinner, the whole cohort always went out and one night we even managed to order a plate of escargots so that everyone could try one. Other culinary highlights were Jacek's steak tartar, many dishes with loads of cheese and, again, the Belgian beer. Although, on the last night we exchanged the beer with rum when celebrating our first and very successful conference trip in a rum bar called La Pirogue.

To conclude, going to the E-MRS Spring Meeting in Lille was indeed a great trip. Together, we had a great time seeing many interesting talks at a very well organised conference and we enjoyed the evenings together in the architecturally very beautiful Vieux Lille. We were also brought together as a cohort, enjoying many fun times which we will remember through our whole CDT experience!

PhD Life

What expectations did you have before joining the TSM-CDT? To what extent have these expectations been met?

I came from a Materials Science background having done a Master's project in materials modelling so I really hoped that the MSc year would help me study important areas of solid state physics, mathematics and computing which are not covered in a materials science undergraduate degree. I felt that the MSc definitely taught me a lot in these areas which I could not see myself as learning if I had gone straight into a PhD. I also found that I learnt a lot from many of the Materials courses because they covered material in a way which was much more mathematical and computational than in my undergraduate degree.
Chris Ablitt (Cohort 6)

I expected the MSc to be challenging with a high calibre of students, providing a useful start to the research project. This has certainly been the case. The combination of taught and research elements in the course has provided a solid foundation for the PhD.
Robert Charlton (Cohort 6)

Describe your project in the simplest sentence you can:

How can Diamond fail?
Mahdieh Ebrahimi (Cohort 4)

I do long simulations once and use them in quick simulations so that I can say I'm saving computational time and will achieve much more than I would otherwise.
Frederike Jaeger (Cohort 5)

Using sunlight to split water at semiconductor surfaces.
Lars Blumenthal (Cohort 6)

I am using computer simulations to help the design of a practical maser (a microwave laser) that works at room-temperature.
Robert Charlton (Cohort 6)

Which experience in the TSM-CDT do you consider to be the most valuable?

Support from all members, including students.
Mahdieh Ebrahimi (Cohort 4)

Personally I think that the Group Programming Project was the most valuable experience throughout the MSc. Working together in a team for such a fairly long time really gave us the opportunity to get to know each other much better and led to significantly stronger bonds between us.
Lars Blumenthal (Cohort 6)

What has been the biggest challenge you have faced in the TSM-CDT?

In the MSc the turnaround between deadlines is often quite tight, as was the time between finishing courses and exams. This meant we were having to process a fair bit of information and tackle tricky problem sheets in a short time. Alone this would have been too much. However, in the CDT everyone worked together on problems - exchanging ideas on a whiteboard and talking over the problems as a group. Since everyone had different backgrounds and strengths, even if you don't feel confident in one area, it's pretty much certain that you will be able to help others in another. It really became clear that working together as a group we were much better than a collection of individuals.
Chris Ablitt (Cohort 6)

Having to make a more long-term research plan after the masters that still contained short-term goals. It required many hours spent reading papers and a LOT of patience.
Frederike Jaeger (Cohort 5)

The biggest challenge was to complete the MSc in TSM. It was a long journey with lots of challenges. I had to focus on the final goal, which was to finish the MSc, in order to overcome this challenge.
Luca Cimbaro (Cohort 6)


Source: L. Blumenthal

Explain who would play the role of you in 'TSM-CDT: The Movie' and why?

A lot of the CDT would probably picture themselves simulating materials in a scene analogous to Ben Whishaw's portrayal of "Q" in Skyfall. The reality is more reminiscent of "The IT Crowd".
Chris Ablitt (Cohort 6)

Ryan Gosling - equally cool.
Vadim Nemytov (Cohort 5)


Source: M. Smith

What would you say to anyone considering applying to the TSM-CDT?

Do it. It'll be one of the best decisions of your life - it'll lead you into a creative and highly satisfying career and professional community.
Vadim Nemytov (Cohort 5)

It is an amazing experience where you learn a lot on both the scientific level and the personal one. I strongly recommend it to anyone who is looking for a challenging experience.
Luca Cimbaro (Cohort 6)

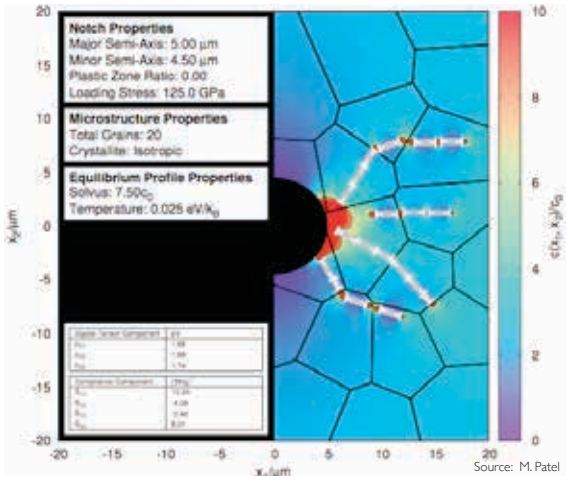
Go, go, go for it! People are really passionate here about TSM and they are eager to find others as passionate as themselves. If you are like this then this is the place for you!
Eduardo Ramos Fernández (Cohort 6)

Delayed Hydride Cracking in Zirconium Alloys

Research Highlight

Mitesh Patel

Nuclear power is a reliable and clean source of energy that offers relatively low CO_2 emissions. As the industry progresses, the issue of safety economics persists and accordingly it is crucial that there is a continued investment in improving the performance of nuclear reactor technology and fuel storage. An important theme is the integrity of the hierarchy of containment barriers designed to prevent the release of radiotoxic material into the environment. One of these barriers is the cladding that encloses the fuel rod assembly; for this purpose, zirconium (Zr) alloys are chosen for their low thermal neutron absorption cross-sections and mechanical properties. However, under operating conditions, Zr is susceptible to a time-dependent hydrogen embrittlement mechanism known as delayed hydride cracking (DHC), the central problem of my research.



Source: M. Patel

The process of DHC begins with an aqueous corrosion reaction at the interface between clad (metal oxide) and coolant water, which introduces hydrogen (H) into the Zr matrix. The H atoms, occupying tetrahedral sites in hexagonal close-packed Zr, diffuse under the influence of the gradients of stress, chemical potential and temperature to accumulate ahead of stress-raiser flaws such as loaded notches. Once the critical concentration of hydrogen is exceeded, "zirconium hydride" precipitate platelets are nucleated. These hydrides are more brittle than the parent metal; they have detrimental effects on the mechanical properties of the component. Any continued application of loading stresses can cause the hydrides to fracture and thereby enable the flaw to propagate. The intertwined repetition of diffusion, precipitation and fracture can ultimately lead to full structural failure.

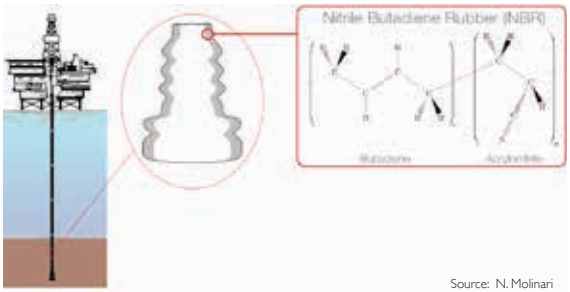
Six decades of industrial and academic research has been directed towards the study of DHC with the overarching aim of quantifying the complexity of the phenomenon. To complement the large volume of experimental work on hydrogen and hydrides in zirconium, my approach is primarily mathematical in nature but now with an expanding computational contribution. My work mainly falls within the 'ancient' (pre-Finite Element Analysis) field of theoretical continuum mechanics; the stress state of the system can be evaluated using various analytical techniques such as the method of elastostatic Green tensors and the method of complex potentials. This information can be supplied into a stress-driven diffusion problem formalised within the framework of linear irreversible thermodynamics through an elastochemical Fickian diffusion potential. Accordingly, hydrogen concentration profiles can be determined and used to investigate precipitation sites; unique to this research is the simplified treatment of the hydrides themselves so as to preserve the analyticity of the calculations. In the background, computational geometry is used to incorporate constitutive rules for hydride nucleation and growth. The upcoming two years are dedicated to developing, verifying and validating this model for industrial use.

Towards a Predictive Model of Elastomer Seal Failure

Research Highlight

Nicola Molinari

Due to their wide and tunable range of properties, elastomers are used in a variety of industries, for example in making seals in the oil and gas industry. In the harsh conditions at which oil wells operate, temperatures up to 500 K and pressures up to 200 MPa can be reached. Under these conditions for long times, the elastomer progressively loses its ability to seal and corrosive chemical compounds threaten to permeate through to the monitoring and telemetry equipment the seal is meant to protect. For these reasons, two scholarships have been offered to the TSM-CDT by a world leading company in the field of oil and gas services, Baker Hughes.



Source: N. Molinari

The first student to start working with Baker Hughes, Musab Khawaja, is focusing on the chemistry of the problem. After creating a fully atomistic description of one of the most common elastomers in the field, Nitrile Butadiene Rubber, he focused on chemical-related properties like solubility, diffusivity and permeability of different gases. Musab has been able to show why CO_2 has a higher permeability than helium (He), despite its greater size. The permeability is the product of the diffusivity and solubility. The diffusivity of He is one order of magnitude higher than CO_2, due to its small size, but CO_2's electrostatic quadrupole means its solubility is two orders of magnitude higher than that of He. By analysing the pore size distribution in the system, he was able to show how these considerations change as a function of pressure. Due to its molecular volume, the solubility of CO_2 falls quicker than He since the pores are shrunk by the increase in pressure. Future work will involve the study of these gases interact with the surface of the seal.

The second student awarded with a Baker Hughes studentship, Nicola Molinari, is focusing more on the mechanical properties of the seals. The starting point of his work was to modify the atomistic description developed by Musab in order to mimic a chemical reaction that industry uses to hydrogenate and cross-link polymers. He evaluated the model by comparing bulk properties like density and glass transition temperature to experimental data. Despite reproducing the correct trends, this analysis highlighted the limitations of the fully atomistic approach when studying mechanical properties. Furthermore, the close collaboration with the industrial partner highlighted the key role that fillers (nanoparticles inserted into the elastomeric matrix for strengthening purposes) have in determining mechanical response. Due to the time and length scale limitations, these had to be ignored in the fully atomistic description (a one nanosecond simulation that included fillers atomistically would have taken nearly 3 years to complete on a desktop computer!). His future work will focus on the development and testing of a coarse-grained model that will lose chemical accuracy, but enable him to develop an understanding of the mechanical properties of real seals that include fillers, thereby getting one step closer to the ultimate goal of preventing seal failure.

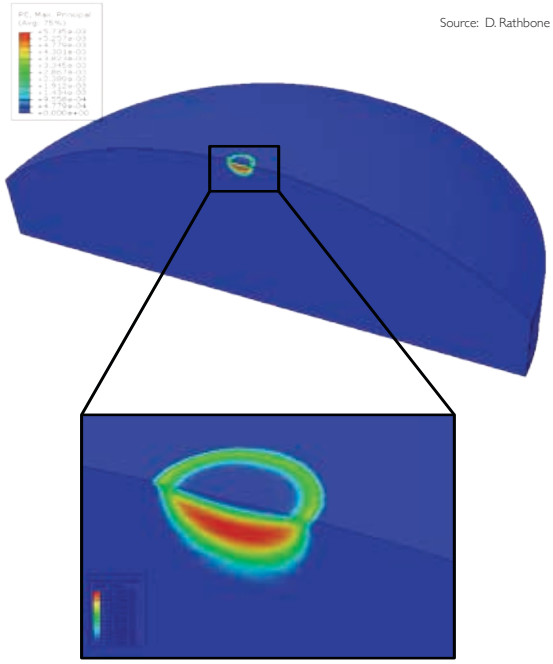
Multiscale Approach to Granular Flow

Research Highlight

DANIEL RATHBONE

GRANULAR MATERIALS are a collection of distinct macroscopic particles such as sand on a beach or salt in a salt cellar. They are of vital importance in many industrial and natural processes, for example, tablet formation in the pharmaceutical industry or avalanches and tidal mudflows. Because of the difficulty and expense of large-scale experiments involving granular flows and the lack of any overarching physical laws to describe them they are ideally suited to computational study. In particular this can be done using the Discrete Element Method (DEM). In DEM the individual grains are treated as distinct particles with a force-displacement model used to describe the forces on each particle when they come into contact. The main advantage of DEM is that it gives information on the microscopic scale of individual particles, which can be used to explore the relationship between macro- and microscopic properties in granular materials. The force-displacement models are fundamental to DEM simulations. The nature of a model and its parameterisation directly affect the accuracy of a DEM simulation.

However, many of the models available in the literature suffer from drawbacks, for example they may be too computationally expensive to use for large numbers of particles or have parameters that need to be found through time-consuming experiments. To overcome these drawbacks we have developed an accurate model for the normal force-displacement relationship between elastic-plastic spheres [1]. By using the finite element method (FEM) we were able to analyse the contact between an elastic-plastic sphere and a rigid plane in great detail in order to develop the new model. We looked at the level of plastic deformation for different material properties in order to develop empirical relationships that relate the parameters of the new model to those properties. This allows the model to be used in DEM for direct simulation of well characterised elastic-plastic materials without fitting parameters to experimental results or doing time-consuming parameter calibration. The model performs better than existing models when compared to FEM results.



Source: D. Rathbone

Since the publication of the paper we have developed a complementary model for tangential forces and we are using it to carry out DEM simulations of the compression of a large number of particles. We hope to validate our model by comparing the results of these simulations to experiments carried out by Johnson Matthey.

[1] D Rathbone, M Marigo, D Dini and B van Wachem, Powder Technology, 282:2–9, 2015.

Hybrid Perovskite Solar Cells

Research Highlight

ANDREW MCMAHON

OVER THE past few years hybrid organic-inorganic perovskites have shown great promise as solar absorbers in photovoltaic cells. Solar cells based on these materials have enjoyed meteoric rises in efficiency in a relatively short space of time, however there remain several underlying questions concerning their physics and operation.

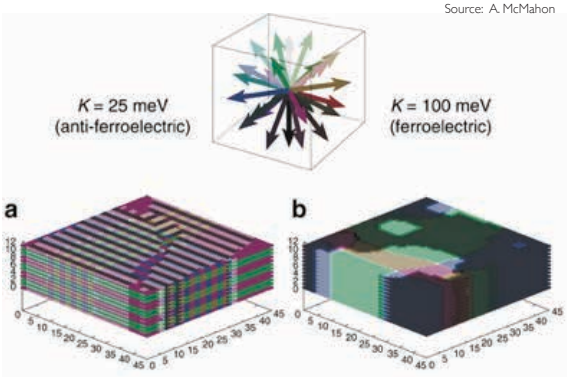
How do these devices behave under an applied voltage? The photocurrent in these devices has been seen to be dependent on the previous bias conditions, known as a hysteresis effect.

The origin of this behaviour is currently unknown, but one hypothesis is that the organic components (methylammonium ions in the case of the hybrid perovskite studied here), which act as rotationally mobile electrostatic dipoles, may rearrange themselves in an ordered fashion similar to dipoles in ferroelectric or anti-ferroelectric materials, which are also hysteretic.

In order to study how the organic molecule in this material behaves, ab initio molecular dynamics calculations and neutron scattering measurements were first performed. This showed that the organic molecules like to 'hop' between different discrete orientations inside the cage created by the inorganic components. These results also showed that the majority of the methylammonium ions were actually not rotationally mobile over a wide temperature range. We hypothesised that this could be due to long range ordering of the dipoles into 'stable domains', which would act to greatly suppress the rotation of the ions.

I then performed a series of Monte Carlo simulations in order to test this 'domain' hypothesis [1]. The simulations were set up in order to 'freeze-in' some domain structures and calculate a defined measure of the probability of rotation throughout the simulation cell. This did indeed show, assuming only electrostatic interactions between the ions, that domains should greatly suppress rotation, with rotation far more likely to occur at the boundaries between domains ('domain walls'). By calculating the change in probability of rotation for the ions after applying an electric field in the simulation, a timescale associated with hysteresis could be derived. This was shown to most likely be too short to be consistent with observed experimental hysteresis.

Source: A. McMahon



These results provide an important addition to the literature and will hopefully stimulate further discussion concerning the role of the organic component in these materials and the role it plays in observed photovoltaic device behaviour.

[1] Leguy, A. M. A. et al. The dynamics of methylammonium ions in hybrid organic–inorganic perovskite solar cells. Nat. Commun. 6:7124 doi: 10.1038/ncomms8124 (2015).

A Fast Orbital-Based Ab-Initio Approach for Ultrafast Dynamics

Research Highlight

MAX BOLEININGER

UNDERSTANDING MOLECULAR orbitals on the femtosecond (10^{-15} s) time scale has long been a dream in science. This timescale involves both nuclear and electronic dynamics, and is hence fundamental for many chemical and physical processes, such as charge transfer, photo-isomerization, and polaron formation, to name just a few.

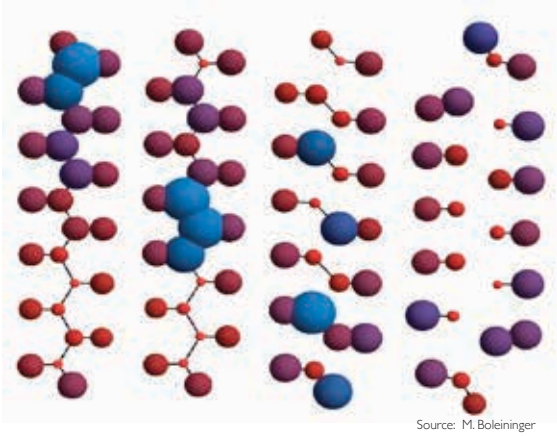
Ultrafast laser pulse experiments are making rapid progress in realizing the technical limits, however obtaining information directly from the experiments about the dynamics of the excited electrons is very difficult. Hence we have to turn to computer simulations. This requires us to develop new computational methods capable of describing matter under the influence of extremely powerful, time-dependent laser fields.

Our method seeks to answer questions such as: can we observe hole migration in organic molecules? Can we tune charge transfer by shaping the laser pulse? What role does nuclear motion play in these processes? Our method hence needs to be capable of describing coupled electron-nuclear dynamics in the time-domain, within strong external fields.

While there already exist models for these systems, such as density functional theory methods (DFT), these are often extremely expensive and require the use of hundreds, if not thousands of computing cores to simulate just a few femtoseconds. We have hence turned our attention on developing a more approximate method based on the density-functional tight-binding approach (DFTB).

DFTB can be seen as an approximate DFT theory, which is orders of magnitude faster by using parameterized matrix elements from single-atom DFT calculations. We however developed a hybrid approach, using an explicit Gaussian basis set.

This allows us to approximate the Hartree and exchange-correlation energy dynamically in relation to the atomic environment, which would otherwise be poorly described in a rigidly parameterised model.



Source: M. Boleininger

We have additionally developed and implemented a formalism capable of describing atomic polarization, which becomes a significant effect under these field strengths – even for hydrocarbons! The same formalism also lends itself well to describe the coupling to an external field. Finally we propagate the electron-nuclear motion in the Ehrenfest approximation, allowing us to account for the momentum-exchange between nuclei and electrons. This adds a basic description of non-adiabaticity to our model.

The resulting method enables us to study these systems in a computationally efficient manner, thanks to a formalism that derives itself systematically from DFT and is hence also systematically improvable. We are now left to apply our method to various organic systems and polymers in strong electric fields.

Authentity

Source: P.Vitelli

Farnaz Ostovari *shares her experience of Authentity, one of the TSM-CDT's residential courses.*

In April of this year, yet another successful Authentity course took place at Cumberland Lodge, which played host to cohort 5 from the TSM-CDT and students from Bristol, Manchester and Sheffield universities. The course is best described by a number of stages; introduction, team building, task delivery and feedback. During the course we were given tasks which were accompanied by masterclasses with the aim of guiding our personal growth both as part of a team and as individual scientists.


Source: P.Vitelli

Students discussing an assignment

We first participated in an 'ice-breaking' exercise where we formed up pairs and had to find out about our partner's hobbies, how they felt about working in a group and what they were expecting from the course. We then had to form a larger group of 7-8 people and introduce our partner to them!

As we became more familiar with each other, each group was put through a number of outdoor activities, where they were given a chance to assess their performance and discuss ways of improving it for the next challenge. Every activity was designed for a specific set of skills, showing that the same group has a different dynamic in various situations; in some cases they succeed and the process is smooth and in some cases this does not hold. One important lesson for me at this stage was that good communication and awareness is a key to an efficient and productive team.

As the course progressed, we were asked to choose one of the major problems in the UK such as "transport infrastructure", "global warming" and "food security" and present our solution in the form of an informative and short video. This was an opportunity for the groups to apply the skills they had learned up to this point and successfully work as a team.

The last stage of the course was focused on the importance and delivery of constructive feedback, which was taught in the last masterclass and applied through one-to-one feedback sessions between the members of each team.


Outdoor group challenge

Source: P.Vitelli

The important lesson for me here was the significance of efficient communication and giving and receiving constructive feedback, both as an individual and as part of a team.


Source: F. Jaeger

Pint of Science

Frederike Jaeger *reports on her experience of the student-led initiative to get scientists and interested members of the public talking over a pint.*


Source: F. Jaeger

Frederike at the pint of science 2015

May 2015 saw yet another instalment of everyone's favourite outreach event, Pint of Science – mainly popular because it takes place in a pub. This year the three day event was held at the Durell Arms in Fulham, picked by yours truly, as it has a rather nice selection of beers with a large and comfortable space at the back, ideal for bringing science to the masses.

This sold out event was the contribution of Imperial's physics department to Pint of Science, a new global event held in 9 countries and 50 cities. The main objective is to give the interested layperson an opportunity to learn more about science in a relaxed and fun setting.

This is why we picked charismatic and engaging speakers from Imperial's finest to tackle the rather broad topic of 'Atoms to galaxies'. Talks ranged from "how to finally get fusion to work" as a viable energy source, via "all things nano" to the beginning of the universe, and I'm proud to say that one of our speakers (Arthur Turrell) made it onto BBC Breakfast for a promotional feature. Each evening started with some good old-fashioned science busking, where the TSM students engaged the curious attendees with science demonstrations such as non-Newtonian fluids (cornflower can do amazing things), bacteria magnification using a laser and 'invisible' balls (which also have the nice side effect of making nappies work). The event was rounded off with a quiz that was enjoyed by all – particularly the movie equations – where being a scientist didn't actually give you much of an advantage.


Source: F. Jaeger

Arthur Turrell talking about fusion

Overall this was a successful event and as an attendee and organiser alike, it was a lot of fun to take part and I'm already looking forward to PoS 2016.

Brixton Science Club

Beth Rice *from TSM cohort 5 shares her experince of helping run a girls only science club in Brixton.*


Source: Flickr--David Jones

The underrepresentation of women in science is an issue many people are working to solve. Some people suggest that the idea that "science is not for girls" sets in early and with that in mind I set up a science club for girls aged 6-10 in Brixton. It takes place at the Baytree Centre, which is an education and social inclusion charity for women and girls in the local area.


Source: B. Rice

Beth helping a student at one of the Brixton Science events

The aim of the club is to get the girls involved in hands on science activities to encourage them to ask questions and get excited about science. We have made 5 minute ice cream to show how salt lowers the melting point of ice, mixed oil and water to make a "lava lamp" (6-10 year olds don't know what a lava lamp is...), used red cabbage as a pH indicator for common household items, investigated polymer science by making slime and built parachutes to see how air resistance works, to name just a few.


Students performing an experiment

Source: B. Rice

The club is volunteer-run and since setting up in 2013, we have had volunteers who are astrophysicists, microbiologists, ecologists, physicists, chemists, neuroscientists and more. Some of the volunteers are students at Imperial, but we have also had people who work at the Society of Biology, the Discovery Channel and in wildlife conservation, which gives the girls an insight into the range of different jobs and subjects a scientist can do.

We hope the club will give the girls an interest and enthusiasm for science that will stay with them as they go through their lives, as well as showing the many different types of scientist they can aspire to be.

Internship at Bosch

Source: A. Greco

Andrea Greco *talks about his internship at Bosch.*

One of the biggest challenges for 21st century materials scientists is the development of new compounds to be used to store and/or convert energy coming from different sources.

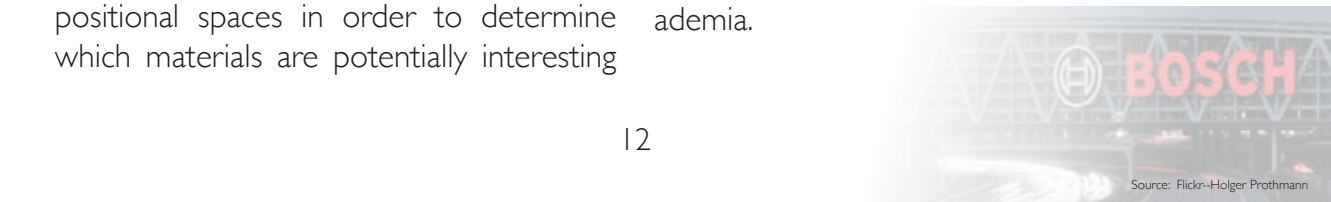
An example is given by the recent effort to switch from fossil fuels to electricity as the main energy source used in transportation. The key for the long-term success of this strategy is the development of reliable batteries that must be able to safely operate under a broad set of conditions and at the same time guarantee long driving ranges without affecting the car driveability (i.e., they have to be embedded in a light and compact package).

I had the very exciting opportunity to work at Robert Bosch LLC in Boston for 6 months. Bosch is one of the companies more involved in the study and development of technologies to be used for the production of next-generation batteries.

My work has focused on the development of automated workflows based on ab initio methods (mainly DFT) to allow for a fast and efficient screening of huge compositional spaces in order to determine which materials are potentially interesting for battery applications. The project was focused on solid-state lithium-ion batteries that have the potential to offer increased safety and durability when compared to liquid-electrolyte based ones.

Materials screening based on ab initio methods is required because of the large number of potentially interesting compounds, combined with the usually complex interactions between the properties of such materials. A trial and error approach based on the experimental testing of each possible candidate would be unfeasible in terms of both time and money. The methods I implemented could help to refine the search for solid electrolytes, that in turn could speed up the development of fully functional solid state lithium-ion batteries, greatly benefitting the electrification of the transport sector.

This experience was very useful for me not only because of the many different methods and approaches I have become familiar with, but especially because I had the opportunity to carry on research in a different environment than academia. I realized how one of the world's largest companies actually takes fundamental research in high consideration, and this opens many exciting opportunities for all the TSM people who are looking for a future position not in academia.



Source: Flickr--Holger Prothmann

***Drew Pearce**, as the leader of the organising team, introduces us to Hermes 2016.*

What makes a successful PhD student? We believe it is high quality skills in your field, excellent communication skills, proficiency in leading technologies and an international network of peers. At the Hermes summer school we aim to provide training and opportunities in all these areas. We bring together leading academics in materials modelling, top science communicators and leading data visualisation specialists to teach and to work with students over the course of their stay. Participants come from top institutions across the globe and over the five days create a lasting network of early career scientific researchers. During the school they work together in groups, utilising their newfound skills to produce a scientific visualisation and explain it at a widely accessible level.


Source: M. Coury

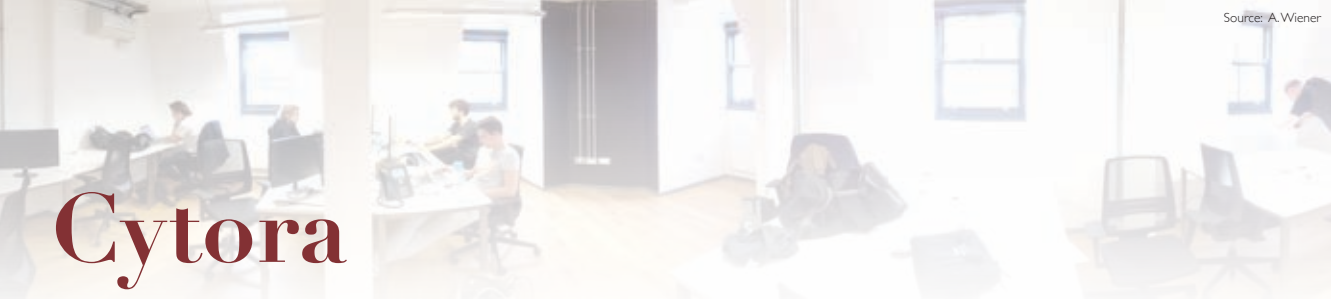
A group activity at Hermes 2014

Hermes 2016 has already been in the works for over a year and there are still nine months before the event itself. We've gone from big undeveloped ideas to having confirmed speakers, secured funding from different sponsors and a preliminary programme. We are still hard at work finalising the keynote speaker and refining the science visualization task in order to ensure the whole event is perfect by the **27th July 2016.**


Source: F. Ostovari

Cumberland Lodge

Hermes has been designed from the ground up by PhD students for PhD students with the aim of providing them with what they want and need, regardless of their career aims. Participants will come away from Hermes feeling more confident about moving forward in their careers, have research skills at the forefront of their field and will have gained world class skills in data visualisation and science communication. How do we know this? All of the Hermes organising committee are previous participants.



Source: A. Wiener

Cytora

Aeneas Wiener, *alumnus from TSM cohort 1 discusses setting up his own tech company.*

At my startup company, Cytora, we monitor open-source intelligence sources for early indicators of geopolitical risk.

I co-founded Cytora together with three friends from UCL at the end of my PhD from the TSM CDT. Since then it has been an exciting adventure to see just how much of my experience as a postgraduate researcher was directly transferable into a high tech startup context. For example, when building our distributed computer infrastructure I was able to draw on experiences from running my own Physics simulations on clusters and HPC workstations around Imperial. This background has given me useful intuition to design our current architecture at Cytora, where we handle thousands of documents per second in streaming mode. This has also been extended to the injection of multi-terabyte historical archives which we use to assess geopolitical risks over multi-decade timescales.

My courses in physics and mathematics, alongside the research experience from my PhD, have also made it easy for me to get up to speed with current research in artificial intelligence and natural language processing, which we use at Cytora to turn completely unstructured text from the open web into structured events, giving us a machine readable stream of what happened, where and when. This stream of risk events is what we expose to our clients from the finance, insurance, defence and aviation industries. For example, one international airline we work with uses our data to monitor the web for mentions of specific risk events around airports that are relevant to the safety of their staff and passengers. The real-time nature of their business means that we had to invest a lot in high-performance processing of information, utilising technologies like C and Cython to ensure sub-second latencies when identifying risk signals from the tens of thousands of streaming unstructured text sources we monitor.

At Cytora we believe that there is tremendous opportunity in observing the world using algorithms. Especially combined with 'internet of things' based information such as temperature measurements or location data, this will bring unparalleled opportunities in understanding and ultimately anticipating human behaviour, from small scale protests outside airports, all the way to macro-level trends such us refugee movements. We are funded by Parkwalk Advisors and Cambridge Enterprise. For current job openings please see our website www.cytora.com and email your CV to aeneas@cytora.com.

Source: Flickr--get down

REROO

By Thomas Edwards

A few years ago I switched from scripting in bash to python for running simulations. Soon I found out about all the cool things you could do with python, such as making web servers and apps. I absorbed the hacker culture at Imperial and started attending hackathons (app development competitions). In February an email caught my eye: Hacktrain, Europe's first hackathon on a train! So I applied of course and I didn't regret it!

Source: T. Edwards

Thomas and his group working on the train

The weekend long event started in London and while on the train we stopped at Sheffield, York and Edinburgh. At Edinburgh all 40 participants spent the night in one room. I even used the carpet as a sleeping bag! My team consisted of the most unlikely gathering of people: 1) Haider, the entrepreneur, this hyper northern lad; 2) Ulrich, the designer, a suave dude from the French Caribbean; 3) George, the mobile developer, plane spotter and student and; 4) myself, the algorithm developer, a TSM geek!

There were some far out ideas, e.g. Tinder for trains but we decided to tackle a more pressing need: expensive UK train tickets. One can save money by 'ticket-splitting', buying two tickets with a total price less than one through ticket. Our aim was to exploit split-ticket savings and offer automated alternative routes (re-routing). For the algorithm, the stations were represented as nodes in a weighted graph, each edge assigned a price. Initially, we used the Dijkstra Algorithm for calculating the cheapest path from A to B but time-dependent prices made things complicated. Nevertheless, having only a proof of concept, we came first and won a plane trip to South Korea for a global hackathon! Unfortunately, it got cancelled due to the MERS virus. However, we got press attention and with our prototype validated, we set out a plan to release by October.

Source: T. Edwards

Thomas and his group holding the trophy of the Hackatrain competition

Working with the train industry was a nightmare. To sell tickets one has to go through lots of red tape to licence your app and make sure you are giving customers valid routes and tickets, which requires paying consultancy fees of about £1000 a day for months. With some outside help we managed to sidestep some of this bureaucracy and come up with a minimum viable product (MVP). Through the hard work of my amazing team we are now on track to release this winter!

www.reroo.co.uk ,@go_reroo

Source: Flickr–Paul Saad

Andrea Greco *reports on his experience at the African school on "Electronic Structure Methods and Applications".*

The 3rd African School on "Electronic Structure Methods and Applications" (ASESMA) was held in Johannesburg (South Africa) from 19th to 30th January, 2015.

This biennial event brings together researchers from all countries, but it is aimed at candidates from the African continent.


Source: A. Greco

A zebra posing for Andrea.

Each student, according to their education and academic career, had the opportunity to explore or delve deeper into three main topics within the ab initio electronic structure framework: optical properties with time-dependent DFT and GW methods, Quantum Monte Carlo methods and Molecular Dynamics.

Each topic was examined thoroughly following a hands-on approach. The students were first introduced to the theoretical aspects by one or more experts in the field, and were then encouraged to perform actual simulations in computational sessions using state-of-the-art electronic structure codes.

I had the honour to be chosen to be part of the team of tutors who helped to design the computational sessions, focusing on ab initio molecular dynamics. All the time spent studying the topic in my TSM career surely paid off in this regard! It made it easier to interact with the students, since the difficulties encountered when setting up my first simulations were still fresh in my mind! Observing the students' progress under our supervision was certainly very rewarding, as was the keen interest they showed in becoming familiar with electronic structure methods.

Overall I really enjoyed my experience at ASESMA. The highlights included the opportunity to help young students to gain a better understanding of what is hidden behind electronic structure methods, and the possibility to explore a culture so different and intriguing.

I would certainly recommend this experience to any colleague in the TSM! The next edition of ASESMA will take place in Ghana in September 2016: please get in touch if you are interested in the amazing opportunity of being part of the team of tutors!

Source: Flickr-James St. John

Materials Challenge Lecture

Mahdieh Tajabadi Ebrahimi *shares with us the highlight of the annual Materials Challenge Lecture and masterclass.*

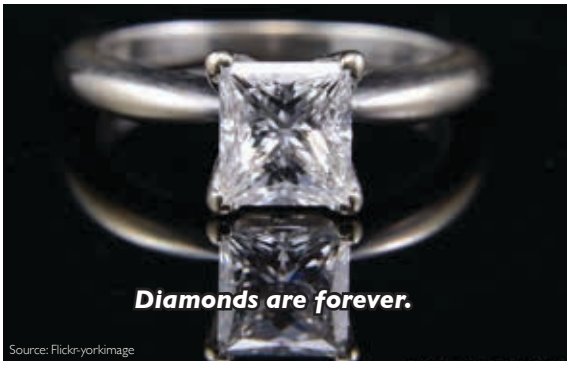
The TSM-CDT was delighted to welcome Dr Serdar Ozbayraktar (pictured below) to Imperial College this June. Dr Ozbayraktar is a Core Technology R&D Manager at Element Six where he started his career in the computational modeling section in 1995. He received his PhD in Metallurgy and Materials Engineering from the University of the Witwatersrand in 1991.

Source: http://www.bitcongress.com/nano2014/program_6.asp

He manages and coordinates various interdisciplinary and multinational materials research teams, product design, conducts energy audits, and runs development projects. These projects are interfaced and partnered with local and international customers, institutes and universities in the United States of America, United Kingdom, Germany, Sweden, Ireland and South Africa.

Dr Ozbayraktar is currently leading material scientists, physicists, chemists, engineers and technologists to design and develop high-performance cutting and machining materials based on synthetic diamond and cubic boron nitride. His specialties are in the field of Metallurgy and Materials Engineering, and microstructural properties of metals and ceramics.

He delivered a Materials Challenge lecture on Diamond Science and Technology, and a masterclass at Imperial College. The lecture covered a brief introduction to the history of Element Six and Synthetic Diamond. The company De Beers Industrial Diamond was founded in 1888 to concentrate on the industrial applications of natural diamond. In the 1960s, the company offered a range of synthetic diamond grit products manufactured by high-temperature and high-pressure processes. In 1992, synthesized diamond films were produced using the chemical vapour deposition technology.



Source: Flickr-yorkimage

In 2002, the company name was changed to Element Six and the production focus directed towards generating diamond for advanced materials applications. In 2013, Element Six launched the Global Innovation Centre in the UK (near Oxford) to develop synthetic diamond and related super-material products for industrial customers in different fields. Products range from oil and gas drilling to precision machining and electronics.

PCD cutter for oil and gas

The theory and practice of synthesizing single crystal and polycrystalline diamond (PCD) were explained in detail. PCD is produced as micron-sized synthetic diamond powders bonded together by sintering at high pressures and temperatures and aided by solvent metal catalysts. Single crystal diamond exhibits different properties in different crystallographic directions, whereas the polycrystalline structure exhibits uniform properties in all directions. This uniformity provides a greater resistance to cleavage and consequently, a stronger material.

PCD discs must be carefully engineered if they are to be used for the demands of specific cutting applications. The current state of multi-scale modelling at E6 was presented, including its impact on material, product and process design, and applications of synthetic diamond.


Dr Ozbayraktar talking about the history of Element Six

He discussed how size and sector of a company affects the working environment, whilst also focusing on the importance of a good work-life balance. Finally he outlined different strategies to establish and improve your position in your job. Overall, the event gave an insight into the world of industry and encouraged us to consider whether we would like to work in a non-academic environment after our PhDs.

Drilling equipment for oil and gas applications

Showcasing success

Annual TSM-CDT Conference

Hikmatyar Hasan *and* ***Lars Blumenthal*** *report on the CDT's very own world-class conferences.*

After having been a great success last year, the student-led TSM-CDT conference took place for a second time this year. Members of staff, the international advisory board and students of the TSM-CDT came together to learn about the achievements students in Cohorts 3, 4 & 5 had made during the previous year. Just as for the conference's debut, all cohorts contributed to a very delightful and interesting get-together.

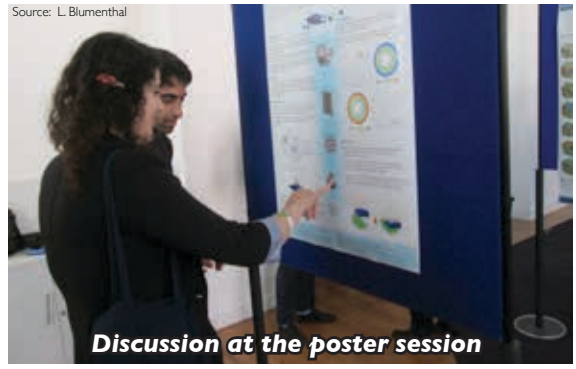
While Cohort 3 presented their research progress individually in 20-minute talks and therefore delivered the main part of the conference, Cohorts 4 and 5 enriched the coffee and lunch breaks with posters about their research. Last but not least, Cohort 6 had the enviable task of rating the posters and talks to decide which of them were prize-worthy.

Source: L. Blumenthal

Prize winners from Cohort II

Musab Khawaja's talk about a molecular study of the gas solubility in nitrile rubber did not only give rise to discussions about whether or not someone's eyeballs would indeed pop when taking a walk in space without a spacesuit, but also won the 'best talk' prize. According to the infallible judgement of Cohort 6, Amanda Diez won the best poster on 'Structures and Processes in a Quantum Rattle'. In an illustrative way she described her work on hollow silica nanoparticles containing clusters of gold atoms which could be used for drug delivery.
An exceptionally entertaining and humorous keynote by Prof. Sergei Dudarev on the problems associated with radiation damage in metals concluded the TSM-CDT conference.

Source: L. Blumenthal



Discussion at the poster session

Three months later, it was the turn of Cohort 6 to present the early stages of their own research at the MSc conference. The results looked promising and surely we will see many exciting posters on their progress at next year's TSM-CDT conference. Although there were no prizes this time, the talks were marked by a highly decorated jury including Prof. Carla Molteni who was invited by Cohort 6 to give the closing keynote talk. Indeed, she gave a very detailed overview of the many different and intriguing fields of her active research. Her particular focus was on pressure-induced structural phase-transformations in nanomaterials.


Source: F. Ostovari

Alumni

Fabian Renn and Valérie Vaissier joined the TSM-CDT in 2010, graduated last year and now…

FABIAN *is a programmer for a popular digital signal processing (DSP) framework called JUCE. Additionally, he and another alumnus of the TSM-CDT (Tom Poole) are the founders and CTO of a small audio effect plug-in company called Fielding DSP. When asked about the role of the TSM-CDT in his current status, he said: "Digital signal processing is all about the responses of discrete time systems and I learned a tremendous amount of the theory of these systems as I investigated methods to describe dielectric material responses with a time-domain computer code." Having left the TSM-CDT, what Fabian misses the most is the interesting, smart and fun people; as he calls them "a great bunch".*

VALÉRIE *is working on methods to simulate systems in condensed phases with the group of Troy van Voorhis at MIT in the US. This includes QM/MM (quantum mechanics/molecular mechanics) calculations of redox potentials in water and the simulation of ground and excited states. Since moving to MIT, Valérie has missed having a "shield from administrative hurdles!". Her response to how the TSM-CDT helped in preparing her for her current role was that "the CDT gets you exposed to a wide research community, it lets you interact with students and academics from many fields. It eases the transition to a new environment after graduation." Which is why if you are considering applying to the TSM-CDT, she advises you to benefit from the TSM community to set up your own path rather than following someone else's footstep as is often the case in a regular PhD programme.*


Source: F. Ostovari

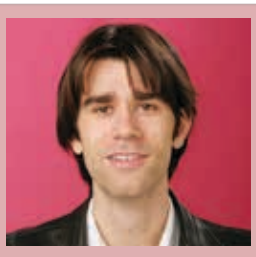
Alumni

A selection of the alumni and where they are now...

Dr Jassel Majevadia
is currently working at IBM as a technical consultant in their Big Data and Analytics service line.

Dr Jawad Alsaei
is currently working at the University of Bahrain as an assistant professor.

Dr Richard Broadbent
is currently working at Rolls-Royce Plc., designing fatigue models for nickel and titanium alloys in the gas turbines.



Dr Anthony Lim
is working for Osaka University and UCL on photon induced phase transformation.

Dr Joe Fallon
is now a data analyst at HMRC, applying cutting-edge data science techniques to generate new insights from the large volume of data.

Dr David Edmunds
is currently doing a postdoc at Royal Marsden NHS Trust in developing software for analysing risks associated with radiotherapy treatment for cancer.

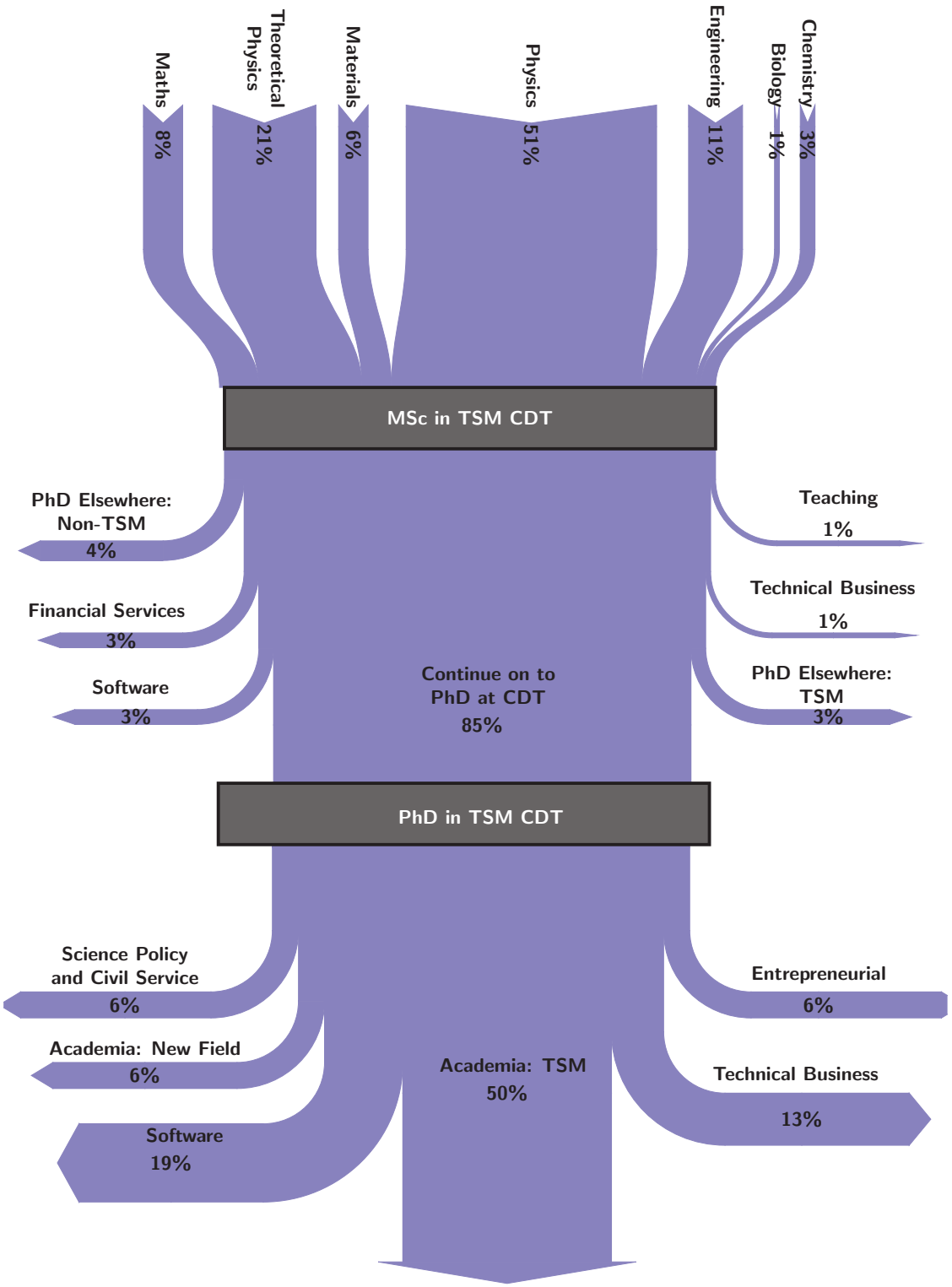
Dr Aeneas Wiener
is now the Co-founder at Cytora where they provide real time data analytics for geopolitics and security threats. (ps: They are hiring)

Dr Niccolò Corsini
is now doing a postdoc with Prof. Matthew Foulkes, studying defects in diamond using DFT and QMC.

Dr David Trevelyan
is currently working at a start-up called Jukedeck, where he is working on artificially intelligent software that automatically composes and produces music.

Alumni - TSM-CDT Graduates: Directions

TSM-CDT student origins and destinations, organised by undergraduate degree and first position after attending the CDT.



Selected Student Publications

An Accurate Force-displacement Law for The Modelling of Elastic-plastic Contacts in Discrete Element Simulations. **Rathbone, D. ;** Marigo, M.; Dini, D.; and Van Wachems, B., ***Powder Technology***, 282 (September 2015)

Theory of The Deformation of Aligned Polyethylene. **Hammad, A.;** Swinburne, T. D.; Hasan, H.; Del Rosso, S.; Iannucci, L.; and Sutton, A. P., ***Proc. Roy. Soc. A***, (August 2015)

The Dynamics of Methylammonium Ions in Hybrid Organic–inorganic Perovskite Solar Cells Aurelien. Leggy, M.A.; Frost, J. M.; **McMahon, A. P.;** Sakai, V. G.; Kockelmann, W.; Law, C. H. ; Li, X.; Foglia, F.; Walsh, A.; O'Reagan, B. C.; Nelson, J.; Cabral, J.T.; and Barnes, P. R.F., ***Nature Communications***, (July 2015)

Current Through a Multi-lead Junction in Response to an Arbitrary Time-dependent Bias. **Ridley, M.;** MacKinnon, A.; and Kantorovich, L., ***Physical Review***, B 91, 125433(March 2015)

Thermally-activated Non-Schmid Glide of Screw Dislocations in W using Atomistically-informed Kinetic Monte Carlo Simulations. Stukowski, A.; Cereceda, D.; **Swinburne, T.D.;** Marian, J.M., ***International Journal Of Plasticity***, (October 2014)

A comprehensive list of student publications can be found at
http://www3.imperial.ac.uk/theoryandsimulationofmaterials/research

2015 Awards

Sutton Prize
Gleb Siroki

Materials Design Graduate Research Prize
Nicola Molinari

Materials Design Advanced Graduate Research Prize
Max Boleininger

Outreach Prize
Frederike Jaeger

Major Contribution to the Life of the TSM-CDT Prize
Frederike Jaeger & Robert Wilson

Julian Walsh Prize for Outstanding Contribution to the TSM-CDT
Farnaz Ostovari

Johnson Matthey Prize for the Best PhD
Thomas Swinburne

Source: Flickr-- Scott Maxwell

Source: F. Ostovari

Current Students and Research Projects

Cohort III

Vincent Chen—*Simulation of the Solid/liquid Interface for Chalcopyrite Leaching (with funding from Rio Tinto)*

Dr Patricia Hunt (Chemistry), Prof. Nicholas M. Harrison (Chemistry)

Marc Coury—*Evolution of Non-Collinear Cagnetism in Hot Iron*

Dr Andrew Horsfield (Materials), Prof. Matthew Foulkes (Physics), Prof. Sergei Dudarev (CCFE), Dr Pui-Wai (Leo) Ma (CCFE)

Thomas Edwards—*Modelling Core-Shell Nanowire Solar Cells*

Dr Andrew Horsfield (Materials), Prof. Nicholas M. Harrison (Chemistry)

Ali Hammad—*Investigating a Molecular Mechanism of Viscoelasticity in Aligned Polyethylene*

Prof. Adrian Sutton (Physics), Prof. Lorenzo Iannucci (Aeronautics)

Benjamin Kaube—*Plasmonics, from Electrons to Devices*

Dr Andrew Horsfield (Materials), Prof. Mark van Schilfgaarde (KCL - Physics)

Musab Khawaja—*Towards a Predictive Model of Elastomer Seal Failure (with funding from Baker Hughes)*
Dr Arash Mostofi (Materials/Physics), Prof. Adrian Sutton (Physics), Dr David Curry (Baker Hughes), Dr John Stevens (Baker Hughes)

Gabriel Lau—*Droplets: from Molecular Nanoclusters to the Atmospheric Aerosols*
Prof. George Jackson (Chem. Eng.), Dr Patricia Hunt (Chemistry), Prof. Ian Ford (UCL - Physics)

Joel Posthuma de Boer—*Epitaxial Graphene*

Prof. Lev Kantorovich (KCL - Physics), Prof. Dimitri Vvedensky (Physics), Prof. Ian Ford (UCL - Physics)

Daniel Rathbone—*A Multiscale Approach for the Development of New Constitutive Laws for Granular Flows*
Dr Berend Van Wachem (Mech. Eng.), Dr Daniele Dini (Mech. Eng.),
Dr Michele Marigo (Johnson Matthey)

Christopher Rochester—*Dynamics of Ionic Liquids in Confinement and the Performance of Ionic Liquid Based Electroactuators*

Prof. Alexei Kornyshev (Chemistry), Dr Gunnar Pruessner (Mathematics)

Cohort IV

Max Boleininger—*Ultrafast Laser Interactions with Thin Polymer Films (with funding from US AFRL)*
Dr Andrew Horsfield (Materials), Prof. Jonathan Marangos (Physics),
Prof. Peter Haynes (Physics/Materials), Dr Ruth Pachter (US AFRL)

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

Dr Edo Boek (Chem. Eng.), Dr Fernando Bresme (Chemistry)

Andrea Greco—*Theory and Simulation of Complex Oxide Materials (with funding from Argonne National Lab)*
Dr Arash Mostofi (Physics/Materials), Dr John Freeland (Argonne National Lab.)

Chiara Liverani—*Quantum Effects in Hydrogen Embrittlement*

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

Adam Ready—*Why is Ti6242 Susceptible to Cold Dwell Fatigue, but Ti6246 Is Not? (with funding from Rolls-Royce)*
Prof. Adrian Sutton (Physics), Prof. Peter Haynes (Physics/Materials),
Prof. David Rugg (Rolls-Royce)

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

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

Mahdieh Tajabadi Ebrahimi—*Multiscale Investigation of Failure in Bonded Diamond Aggregate (with funding from Element Six)*
Dr Daniele Dini (Mech. Eng.), Dr Daniel Balint (Mech. Eng.),
Prof. Adrian Sutton (Physics), Dr Serdar Ozbayraktar (Element Six)

Robert Wilson—*A Multi-Scale Approach to Understanding Cohesive Particle Flows*
Dr Daniele Dini (Mech. Eng.), Dr Berend Van Wachem (Mech. Eng.), Dr Michele Marigo (Johnson Matthey)

Cohort V

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

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

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

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

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

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

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

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

Andrew McMahon—*The Behaviour of Charged Species in Hybrid Organic-Inorganic Perovskite Photovoltaics*
Prof. Nicholas M. Harrison (Chemistry), Dr Piers R.F. Barnes (Physics), Prof. Joost VandeVondele (ETH Zürich - Materials)

Nicola Molinari—*Towards a Predictive Model of Elastomer Materials (with funding from Baker Hughes)*
Dr Arash Mostofi (Materials/Physics), Prof. Adrian Sutton (Physics), Dr David Curry (Baker Hughes), Dr John Stevens (Baker Hughes)

Vadim Nemytov—*Nanocrystals by Design: Combining the Power of Atomistic Force Fields and Linear-Scaling Density Functional Theory (with Materials Design scholarship)*
Dr Paul Tangney (Materials/Physics), Prof. Peter Haynes (Materials/Physics)

Premyuda Ontawong—*Atomistic-to-Continuum Theory of Martensitic Transformations*
Prof. Dimitri Vvedensky (Physics), Prof. Lev Kantorovich (KCL - Physics), Dr Carla Molteni (KCL - Physics)

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

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

Mitesh Patel—*Multiscale Modelling of Delayed Hydride Cracking (with funding from Rolls-Royce)*
Dr Daniel Balint (Mech. Eng.), Dr Mark Wenman (Materials), Prof. Adrian Sutton (Physics)

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

Prof. Jenny Nelson (Physics)

Beth Rice—*Tight-Binding Approach to the Simulations of the Electronic and Optical Properties of Porous Conjugated Molecular Materials*
Prof. Jenny Nelson (Physics), Dr Jarvist Moore Frost (Bath - Physics), Dr Kim Jelfs (Chemistry)

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

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

Cohort VI

Chris Ablitt—*First Principles Lattice Dynamical Study of Ferroelectric and Negative-Thermal-Expansive Ruddlesden-Popper Oxides*
Dr Arash Mostofi (Materials/Physics), Dr Nicholas Bristowe (Materials), Dr Mark Senn (Oxford - Chemistry)

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

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

Robert Charlton—*Computational Excitonics of Doped Organic Molecular Crystals for a Room Temperature Maser (with an Imperial College PhD Scholarship)*
Prof. Peter Haynes (Materials/Physics), Dr Andrew Horsfield (Materials)

Luca Cimbaro —*Embrittlement of Ni-based Superalloys by Oxygen (with funding from Rolls-Royce)*
Dr Daniel Balint (Mech. Eng.), Prof. Tony Paxton (KCL - Physics), Prof. Adrian Sutton (Physics)

Jacek Golebiowski—*Self-Diagnosing Polymeric CNT Composites – First-Principles Atomistic Simulation of the Effects of CNT Functionalization (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)*

Dr 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 CCFE)*

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*

Dr 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 Science and Engineering)

Cohort VII – A warm welcome!

Ignacio Bordeu (with funding from Conicyt), Harry Cardenas (with funding from Conicyt), Alessio David, Fangyuan Gu, Mariana Hildebrand (co-funded by NPL), Maciej Jarocki, Nuttawut Kongsuwan, Charles Penny (co-funded by STFC), Nikoletta Prastiti, Lara Roman Castellanos, Christopher Sewell (co-funded by BP), Panagiotis Simatos (co-funded by Toyota), Fred Temple, Andrew Warwick.

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Prof. David Rugg – Rolls-Royce
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Prof. Dominic Tildesley – Director of CECAM
Prof. Helena Van Swygenhoeven – Paul-Scherrer Institute & EPFL, CH
Dr Erich Wimmer – Materials Design, Inc.

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Dr Daniele Dini – Cohort Mentor: Cohort III
Dr Daniel Balint – Cohort Mentor: Cohort V
Prof. Mike Bearpark – Cohort Mentor: Cohort VI
Dr Andrew Horsfield – Cohort Mentor: Cohort VII
Dr Simon Foster – Outreach Officer
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For a full list of staff see: http://www3.imperial.ac.uk/theoryandsimulationofmaterials/people/academicstaff

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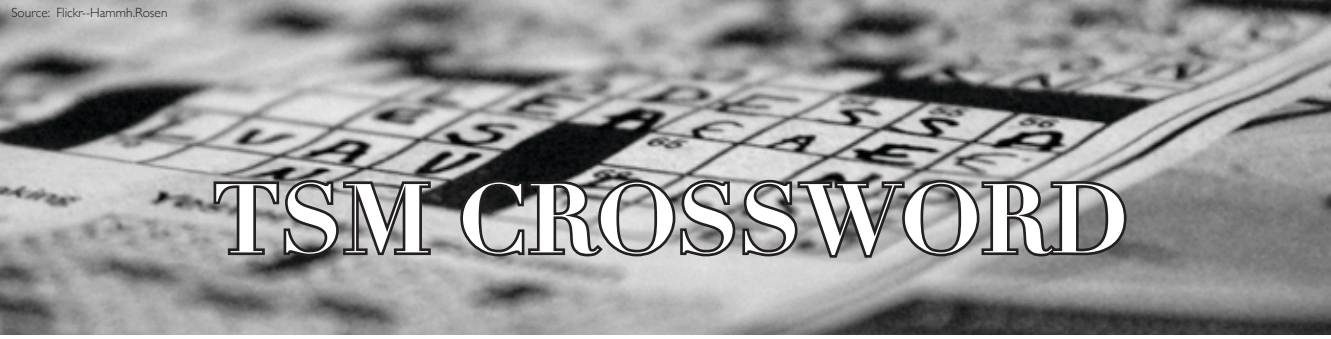
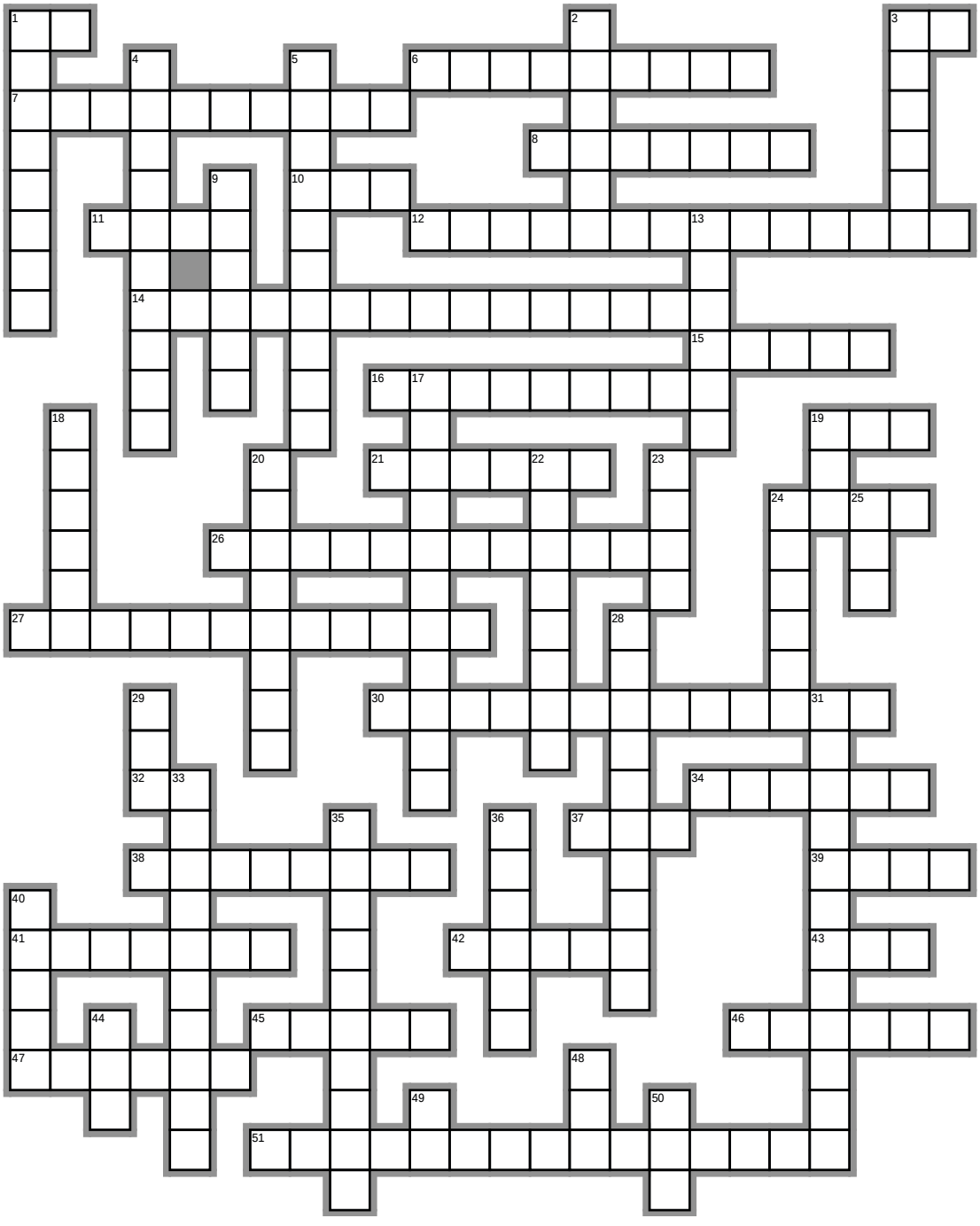
Source: Flickr--Hammh.Rosen



TSM CROSSWORD



Clues across

1. Biggest oil and gas company in UK [2]
3. Coarse Graining (abbreviation) [2]
6. Stretchy seals [9]
7. Our Bread and Butter [10]
8. Admin heroine [7]
10. Us [3]
11. Women in science and Engineering [4]
12. TSM gets festive [9,5]
14. Our home in Windsor Park [10,5]
15. Here comes the sun [5]
16. Mitesh's metal [9]
19. TSM-...? [3]
21. Mostofi, Balint, Dini, ... [6]
24. Material building block [4]
26. The product of our PhD [12]
27. Commercially sensitive data is ... [12]
30. Takes a lot of time [4,9]
32. Molecular Dynamics [2]
34. Outgoing director [6]
37. Regal member of 43 across [3]
38. Scotch-tape and pencils [8]
39. Not quite San Francisco [4]
41. The king of dislocations [7]
42. Spherical cows [6]
43. London's consortium of modelling [3]
45. Bisch, Basch, ... [5]
46. Birthplace of Ada Lovelace [6]
47. City of dreaming spires [6]
51. Sponsor of our Graduate Research Prizes [9,6]

Clues down

1. Steel-master, put Sheffield on the map [8]
2. What's right, what's wrong? [6]
3. An ancient Roman military unit [6]
4. Bridging scales [10]
5. # Current students [5,5]
9. Messenger god [6]
13. Electrons in Africa [6]
17. Introduction activity [3,8]
18. Ab ... [6]
19. Schrödinger's pet [3]
20. TSM's home [8]
22. Simon Foster's domain [8]
23. Really, really small [4]
24. Recovering TSMers [6]
25. Solar panel made flexible [3]
28. Physics meets gambling [5,5]
29. Grains modelled as distinct particles [3]
31. Weird ... fluid (e.g custard) [3,9]
33. Hosted PoS 2015 [6,4]
35. Next generation photovoltaic [10]
36. Disasterous Analytics [6]
40. Scientists in TRAINing [5]
44. "It's a Kohn and a Sham" [3]
48. Professor Adrian Sutton ... [3]
49. 40 Down without the vowels, sponsor of CDT (abbreviation) [2]
50. Required TSM sustenance [3]

Email your solutions to: andrew.mcmahon13@imperial.ac.uk

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