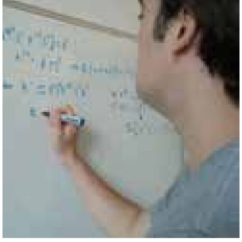
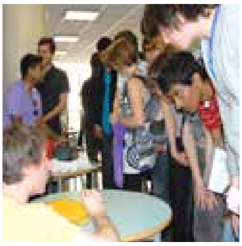





Centre for Doctoral Training on

Theory and Simulation of Materials





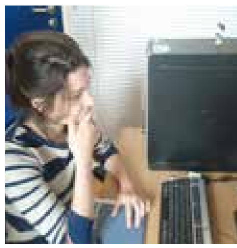










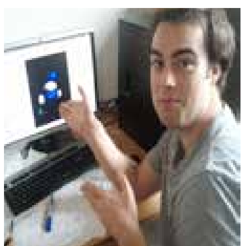



Annual Report

2011–2012









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London, September 2012

Director's Foreword

The Oresund Bridge (pictured left) spans the five mile strait between Malmö in Sweden and Copenhagen in Denmark. Apart from being one of the major engineering achievements of our times, it is remarkable in that it connects two countries with similar cultures and a shared past yet with different languages.

The mission of the Centre for Doctoral Training on Theory and Simulation of Materials (CDT on TSM) is 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. Traditionally, different disciplines have tackled the same problems at different scales. The TSM-CDT seeks to go much further by bridging those scales, explicitly transferring information between them. Like the Oresund Bridge, this involves connecting two territories where the inhabitants speak different languages. There are two key aspects to this bridge-building. First, providing our students with a comprehensive multi-disciplinary training in the form of the MSc on TSM. Second, creating new cross-disciplinary collaborations that have so far involved seven departments at Imperial as well as other institutions, including some of those participating in the Thomas Young Centre - the London Centre for TSM.

The TSM-CDT was founded in 2009 with funding of £6.4M from the Engineering and Physical Sciences Research Council. This October we welcomed our fourth cohort, bringing us to full capacity for the first time. It is therefore an appropriate moment to publish our first annual report. It covers the wide variety of activities that our students

have been engaged with during the 2011-12 academic year.

However, at its heart the TSM-CDT is all about people. That is why we invest significant time, effort and money in our admissions process, cohort-building, mentoring, outreach, as well as developing innovative professional skills training and matching students with research projects. The student experience in the TSM-CDT is not about the staff keeping the students busy, but rather providing them with the time, support and resources to develop the initiatives they want to pursue. That is reflected in this report, which is almost entirely written and produced by a team of students. Whether you are a prospective or a former student, an academic or industrial partner, or just happen to be passing by, I hope you enjoy reading this perspective on life in the TSM-CDT.

Peter Haynes

Contents

"Not the Roman Legion"

The Cohort 3 Student Experience

***Marc Coury**, student representative for Cohort 3, reflects on the experiences of his MSc year and tries to put his finger on what it means to be a TSM student:*

Being a student in the TSM CDT is both challenging and rewarding. You definitely need to work hard. Luckily you have other members of your cohort to help you out when you get stuck. It is rewarding both in a tangible and intangible way: you get a shiny new MacBook Pro when you arrive, free lunches every week and you get taken to a massive conference far away in your first year. At the same time you are given opportunities to learn from some of the world leading academics in materials modelling, the satisfaction of resolving challenging problems and your work has the potential to have real world applications.

This broadens your perspectives: before joining the TSM CDT I was still uncertain exactly what I wanted my PhD project to be on. In the CDT you choose the research project from a large list after 6 months into the course. If you don't like any, you can always propose your own—as I did. Proposing your own project might be difficult, but the CDT offers you a unique environment to make the right choices. One of the most useful intangibles I have received is being offered the broader picture of the current successes and limitations of various materials modelling techniques. In other words, not being limited by the idea that a single simulation technique can solve all problems. I have learned about the successes and failures of multi-scale modelling and, most importantly, that it is the transferral of the physics and the mechanisms from one scale to another that is key to a successful model—not just numbers.

Being in a cohort does not make you a part of the Roman legion. However it does entail training, team work and development in a group of select students. The best thing that we did as a cohort this year was, in my opinion, the group programming project: to write a molecular dynamics tight binding program for carbon. Our codes produced some interesting results on carbon nanotubes and buckminsterfullerenes. Perhaps more importantly though, the experience taught me about the complexities of producing a code in a group, in particular transferral of data between independently coded modules.

Less Pressure; More Coffee

The Cohort 2 Student Experience

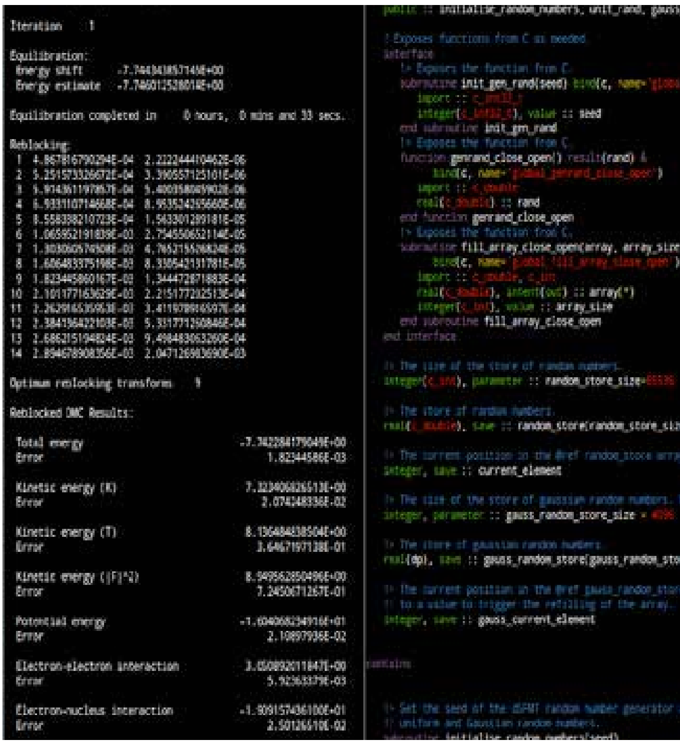
Things get better, reports student representative ***Tim Zühlsdorff*** *(Cohort 2):*

Source: Wikimedia Commons

The second year of the TSM CDT marks the end of the taught lecture courses and the start of the individual research projects. Members of my cohort enjoyed the individual freedom and excitement this time brought. Our supervisors gave us the chance to explore our field of research.

All in all this year was defined by a more relaxed atmosphere, compared to the first one with its timetabled lectures and deadlines. We got the opportunity to pursue our research in different directions without being under pressure to produce significant results right away.

Though we are no longer seeing each other daily, there are still strong ties in our cohort, that manifest themselves in regular coffee or lunch breaks, evenings in one of the many local pubs or even research collaborations. Without these friendships with our cohort colleagues, most of us would have found our first year as PhD students to be an intimidating experience. If there is one thing all of us have learned in our second year on the programme, it is that research can be very rewarding, but also frustrating at times. It is in those frustrating periods that it becomes most helpful to have people around who understand the pain of a crashed simulation or a segmentation fault. So I think it is fair to say that we still benefit greatly from the unique cohort system this course provides us with.



MRS and the US

Cohort 3, Stateside

The MSc student 'conference experience', aka the "go anywhere in the world as long as it's to learn about Materials" trip once again sees a cohort travel to the MRS Spring Meeting. ***Ali Hammad*** *(Cohort 3) reflects:*

Over the week of the 7th–13th April, members of the third cohort travelled to San Francisco to attend the Materials Research Society Spring Meeting. This conference, held annually since 1983, is now regularly attended by over 5,000 participants from research and industrial institutions around the globe. Its 50 or so symposia run in parallel across five days, covering every material aspect of the annual theme–this year was Sustainable Development.

Before venturing into the 5,000 strong mob of material scientists, the cohort was able to use the weekend to settle in. The relaxed *'cali'* lifestyle coming naturally to the jet-lagged students. Sight-seeing and taking in the local food and city life were on the agenda until Monday morning, when the educational aspects of the trip began to be enforced. Accompanied by their cohort mentor, Daniele Dini, the students headed to the Lawrence Berkeley National Laboratory. They received a series of informative talks from its researchers before enjoying an informal lunch. The MRS conference started later that evening with a social event to allow the different attendees to get to know each other.

The students agreed they were completely spoilt for choice with regards to conference talks. Material ranged from research at the atomistic level to the exploration of engineering scales. With plenty of symposia containing topics completely unfamiliar to them, the cohort had to choose their talk schedules carefully.

Plenary sessions, often featuring very high-profile speakers proved a popular choice among the cohort. One such talk, from Koichi Kitazawa of the Japan Science and Technology Agency was about the nuclear disaster in Fukushima. In it, apart from addressing future trends in energy technologies, Kitizawa addressed the shift in research approach Fukushima's disaster signifies for R&D–a move from curiosity-driven to problem-based research.

By the end of the week the combination of hectic talk schedules and San Franciscan nightlife had the students feeling burnt out. Many headed back to the UK when the meeting ended, but for some cohort members, a second trip (to recover from the labours of the first) was in order. They splashed out on a tour of California.

Weird Weekends

Cohort 2 and the Legacy of Authentity II

Convert ***David Trevelyan*** *on The Call of the Weird, or, what really happened on the Authentity (sic)* ***transferable skills*** *course:*

An army of sceptics went in, yet only a handful returned. *Authentity II* blew away the status quo in the understanding of what transferable skills are, what their true value is and most importantly, how they can be learned. April 2012 saw the second cohort of the TSM CDT return, one year after their first-cohort counterparts, to Cumberland Lodge for three days of stress, socialising, and real self-discovery. It was exhausting, at times excrutiatingly uncomfortable, but all agreed it to have been a thoroughly enjoyable experience.

The ground-breaking new course from Piero Vitelli followed a similar path as the previous year. Engaging participants in a real team situation, whereby small groups were to (amongst other smaller tasks) entirely produce a short film designed to promote understanding of the societal benefits of the work of Authentity's partner: the **Bloodhound SSC** project. The real benefit of the course was not, as some might have expected, in learning *how* to work in a team environment. Instead, the students were treated to a uniquely open atmosphere in which they were offered sometimes startlingly pertinent feedback on their demeanour, personality, behaviour and their influence on those around them. Authentity taught not what kind of behaviour to adopt, but instead how to recognise and understand it in oneself and others.

The Bloodhound Project is based on a truly visionary idea: to design and test the world's fastest car and, in so doing, make science and engineering attractive to children. By offering them enough inspiration to make sure that when time comes they choose to pursue a career in any of those fields, the team at Bloodhound SSC seeks to address the deficit in technical thinking among the population. This is indeed a big problem western societies are facing, for the numbers of scientists and engineers are dwindling at the same pace we all realise how fundamentally based on technical expertise our culture and economy is.

The Bloodhound car will be tested in January 2013 in South Africa, and if all goes right will run faster than the speed of love: 1000mph! £15m well spent!

www.bloodhoundssc.com

Careering Ahead

Cohort 1 prepare for life outside the CDT

With only one year of funding remaining, it's probably time for another Transferable Skills Course. ***Rob Horton*** *(Cohort 1) reports:*

From the 28th to the 30th of June 2012 members of the first TSM CDT cohort, along with students from the Institute of Chemical Biology CDT, attended a careers course at the Royal Society's Kavli Centre at Chicheley Hall. The course director was Dr Ann Canham, former VP of Human Resources at BP. The aim of the course was to expose students to the wide range of careers accessible to people with a scientific background. This took place over three days with each day being dedicated to a different aspect of career development.

The first day was devoted to the identification of personal values and the importance of taking these into account when choosing a career. The students engaged in a number of exercises, led by the course tutors, which helped them to analyse what they held to be important and taught them to take these values into account when choosing a career.

The students spent the second day speaking to professionals from a range of industries: Dr Duncan McInnes (Bank of America Merrill Lynch); Prof Lesley Cohen (Head of Experimental Solid State Physics Imperial College London); Alok Jha (The Guardian); Dr Fabio Pulizzi (Nature Materials); Heather Barker (charity sector) and Dr Nick Green (Science Policy, The Royal Society). Initially the students met with the professionals in small groups to allow them to gain an insight into each industry. This was followed by a panel discussion where students were able to raise further questions.

The final day was spent examining the process of getting to interview and interview practice. Elspeth Farrar (Director of the Imperial College Careers Service) held a session outlining the application process. The students then had the opportunity to be interviewed for a chosen role as well as to interview other students allowing them to gain an insight into the whole process. This insight will dovetail into more traditional interview practice, which will take place in November.

Scientific Festivities
TSM at the CDT 'Festival of Science'

*Sermons and soda-water, but also mirth and laughter at a festival Lord Byron's Don Juan could be proud of. Organiser **Joshua Tsang** (Cohort 2) reports:*

The CDT 'Festival of Science' was a student-organised conference that took place on the 30th March 2012. It provided an opportunity for CDT students to confront and engage in critical discussion of issues faced by today's researchers, from open-source publishing to supply and demand in the PhD chain. The conference was unique in that all the events were designed to maximise the attendees' participation, whether this was in chaired think-tank sessions or in the video booth, where students were given one minute to pitch their research.

Prof. Adrian Sutton (TSM Chairman) introduced the day, making TSM's contribution to the proceedings well known. **Sir John Beddington** (Chief Scientific Advisor to the UK Government) then gave a rare glimpse into the challenges faced by a scientist in the corridors of Whitehall—indeed he even illustrated this point when his talk was delayed due to an emergency meeting with the Prime Minister! Sir John drew the perhaps surprising conclusion that the challenges posed by food, water and energy shortages dwarf those given by the then-topical nuclear reactor meltdown at Fukushima for example. Following a lunch break came the ever-popular **Dr Simon Singh** with a first-hand account of his fight against libel charges and for libel-reform. Next, **Dr Simon Chaplin** (of the Wellcome Trust) delivered a fascinating talk on how the public's perception of medicine has changed such that nowadays public acceptance is gained through transparency, and not by doing science behind closed doors. And finally **Dr Cameron Neylon** elucidated the principles and philosophy behind open-source scientific journals.

The volume of input from the attendees was overwhelming, with some of the most interesting ideas expressed by the participants themselves. Attendees pointed out that despite the broad spectrum of disciplines spanned by most CDTs, this spectrum is still finite and can be restrictive. This suggests a need for the continued evolution of the CDT model.

All in all, the atmosphere of the conference was fun and extremely productive. Difficult issues were openly discussed with valuable conclusions drawn. Perhaps the greatest testament to the Festival's success was that discussions continued well after the conference ended into the post-event drinks!

Johnson Matthey Visit

*Cohort 3's **Daniel Rathbone** reports on an industrial visit to **Johnson Matthey**, the British chemicals and precious metals multinational.*

On 15th March Cohort 3 visited Johnson-Matthey at their technology centre in Sonning Common. On first arrival, students were given an introduction to the business. Johnson Matthey is a global company whose speciality is in chemicals, in particular the production of catalysts. R&D plays an important role in their company and within this there is an essential materials modelling component. Modelling can help with the development of new catalysts, for example, designing systems that maximise activity while reducing the amount of precious metals that are needed, thus accelerating the process of generating a new product and bringing it to market.

A definite highlight of the day was a brainstorming session on the two PhD projects being offered in collaboration with Johnson Matthey. The first of these proposed projects would concern the growth of metallic nanoparticles on oxide supports; many catalysts consist of metal nanoparticles on a substrate and these catalysts degrade with time because the nanoparticles grow. Students put forward ideas as to which different aspects of the problem would need to be investigated in order to find the driving force behind this growth. These included the elastic forces between nanoparticles, the amount of particle migration and the role of Ostwald ripening. They saw that there was very broad scope to the project and a real opportunity to make an impact on the understanding of catalyst degradation.

The second, entirely different, project was to involve the development of new constitutive laws for granular flow. Granular flow is the movement and interaction of large numbers of macroscopic particles and is very important in manufacturing processes. The aspects of the collision between two particles that would have to be characterised in order to describe the behaviour of a large number of particles were discussed and it was discovered that the problem is extremely complex, with a large number of variables to consider in just in a single collision. This session gave an introduction to two very different but very interesting projects, both with the potential to make a large impact in their fields. Through the collaboration with Johnson Matthey such academic impacts could feed through very quickly to industrial applications.

Author Daniel Rathbone (Cohort 3) has since taken up the second of these projects. His PhD, "A new model of mechanical properties of aligned polymers", will be completed under the supervision of Dr Van Wachem and Dr Dini (IC Mech. Eng.), as well as two researchers from Johnson Matthey's R&D Department—Dr Michele Marigo and Dr Selassie Dorvlo (Engineering and Materials respectively).

‘Frankenstein Food’ and other Questionable Practices

Cohort 3 sit Research Ethics I (01)

Lessons in Right and Wrong were alright, says ***Vincent Chen*** *(Cohort 3):*

In October, first year students of several Imperial CDT programmes gathered together for a thought provoking one-day course on Research Ethics. The topic of Research Ethics is extremely important as it concerns not only the quality of research, but also the reputation of science in the public view. Led by Oxford University philosopher Marianne Talbot, the course focused on several ethical issues that CDT students may encounter during their research careers.

After a warm up on the basics of research ethics, Marianne dived into the chosen topics one by one. Firstly, they looked at several case studies of notorious research misconduct, pathological science and questionable practices. Then students discussed their consequences and ways to guard against them. Second came a lesson about the business nature of the conventional academic publishing model and the emergence of the alternative open access model. Ways to encourage academics to embrace the open access model were also discussed at this stage. Finally, the CDT students learnt about the negative impact that prevalent (mis-)reporting of science has on the reputation of science itself. A classic example discussed was GM crops which suffered from heavy regulation after the media driven ‘Frankenstein Food’ scare.

‘*Audience interaction*’ was an important part of the course with many students contributing their views and interesting anecdotes to lively discussions throughout the day. By carefully dividing the class into smaller groups to discuss specific issues, Marianne allowed shyer students to play a part in the discussion. This involvement of the whole class was a contributing factor to the success of the course. Overall, it was a very educational day that will help CDT students towards becoming well-rounded researchers, with increased awareness of ethical issues associated with their activities.

Those interested in finding out more about the study of philosophy and ethics can download lectures and podcasts from Marianne’s website, ***www.mariannetalbot.co.uk.*** *In addition to her original podcast successes (3 million iTunes users can’t be wrong!) her newly released book on bioethics—Bioethics: An Introduction—can be purchased from Cambridge University Press.*

The Burden of Proof

More audience participation as Cohort 2 take Research Ethics II

Pyrrhonic sceptic ***Beñat Gurrutxaga-Lerma*** *(Cohort 2) reports on Ethics II, and its reception by an older, wiser, cohort:*

Source: Wikimedia Commons

What is truth? Can it ever be achieved? Are there absolute moral beliefs? Is the precautionary principle always justified, or should we sometimes accept the inevitable risks that come with research? These are some of the topics Marianne Talbot introduced in the second instalment of Cohort 2's Ethics course, which took place on the 14th May.

Apart from being an occasion for a constructive break as the 9 month assessment review of Cohort 2 was approaching, there was a general agreement that the course offered them an occasion to challenge or, at least, reflect on their own beliefs, and learn about the ethical dilemmas they may face in the future.

Marianne took a dogmatic stance which was not always shared by all her public, where pyrrhonic sceptics, cognitive relativists, neo-Platonists, deontologists, postmodernists, logical positivists and existentialists were all present: a rich mixture of philosophies that could only deepen the quality of the thriving (and surprisingly polite) discussions that arose as she guided students through each of the topics mentioned above. Whether or not she succeeded in convincing anyone of the blunders in their beliefs is out of the question, because she never tried such a thing. The ethics course is devised to make students aware of the ethical problems they may face throughout their future (and current) career. Inasmuch as she was able to surface so many schools of thought in the sessions that spanned that day, one could only dub her task as utterly successful. Everyone enjoyed the ethics course and, indeed, everyone is now looking forward to its third instalment.

Beating the Year Two Blues

The Cohort (I) Mentor Experience

The Cohort Mentor scheme, unique to the CDTs, provides a good tonic. ***Dr Arash Mostofi*** *(Deputy Director of the TSM CDT and Mentor to Cohort 1) comments on the impact this post can have:*

This year, Cohort 1 members have been in their second year of PhD research, a time notorious for its "second year blues". It is typically the period in which some of the most difficult obstacles have to be overcome, whether technical or conceptual. It is also the time when the pressures of getting results, analysing and understanding them in depth, together with the looming task of writing a 150-page thesis, can seem all too much.

Cohort 1, however, came up with an idea to help beat the blues. Instead of our usual cohort meetings, members of the cohort volunteered to present a problem that they are currently encountering in their research. Together, the cohort would brainstorm some solutions. I am happy to report that in most cases, at least one or two of the ideas that are thrown around turned out to be very useful!

These problem-solving sessions have an added benefit as well. It comes from the fact that the students in the cohort are doing research on completely different topics and in different departments. This means that they must learn to communicate with one another across the traditional divides that exist between disciplines. This is a key feature of their training in the CDT.

The Cohort Mentor Scheme

One of the key philosophies of the TSM-CDT is for the experience of the students to be strongly cohort based. One member of academic staff is assigned as the mentor for the cohort of students starting the TSM-CDT programme and stays with the cohort throughout the 4 years of training.

The role of this cohort mentor has a number of facets, including welfare and pastoral care, receiving evaluation of the course and providing feedback to the students, and helping to set the general ethos of the CDT. More than an administrative figure, the cohort mentor is an amiable buddying figure that helps to give cohesion to the cohort.

It's Outreach Time!

TSM Students respond to their emails, and get involved with schools Outreach Projects

Outreach Officer ***Dr Simon Foster*** *gives a whistlestop tour of all the outreach activites carried out in the TSM CDT this last year:*

It has been a busy year for Outreach in the TSM CDT with Simon Foster taking over the role of Outreach Officer.

In July the TSM played host to the first CDT 'Experience Day', where physics teachers were invited along to Imperial to get a taste of the research being conducted by the TSM group. Peter Haynes and TSM students gave a series of talks and workshops which immersed the teachers in the work of the group. It allowed them to understand the exciting work being conducted by the group and gave them knowledge to take back into the classroom to inspire the next generation of scientists!

TSM members were also a key factor in the success of this year's Physics Department open days, which took place throughout June. Students conducted exciting live experiments to audiences of over 150 school students, explaining their research in simple and interesting ways which helped to inject excitement and wonder into the open days.

In the same month, the students ran a series of experiments with work experience students who were visiting the Physics department. These experiments gave the students the opportunity to handle equipment and materials that are not usually available within schools.

Throughout the year students have undertaken talks at schools and colleges, discussing the work of the groups as well as promoting physics as a career. Adrian Sutton has developed links with the Phoenix High School in White City. This has lead to a number of events being held at the school, including the successful sixth form debating competition centred on the argument of climate change.

Research Highlight:
Nanofocusing performance of metallic tips

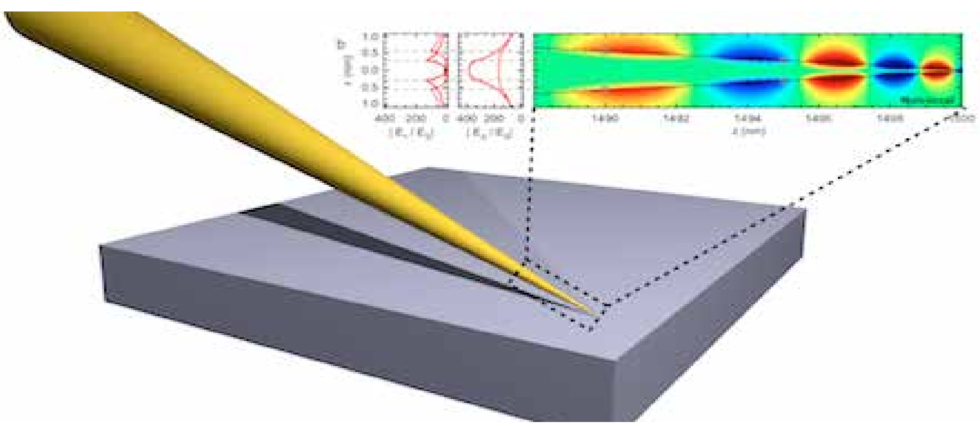
***Aeneas Wiener** (Cohort 1) introduces us to the topic of his latest paper on plasmonics*

Localisation of optical energy into sub-wavelength volumes is currently an active area of research in the field of nano-optics. The challenge arises from the fundamental limitation that a beam of visible light cannot be focused in a spot that is smaller than its wavelength. If achieved, nanofocusing could also be reversed, so that it could act as a sensor for electromagnetic signals with nanometer accuracy, something highly desirable for the study of chemical reactions.

From the point of view of multi scale materials theory and simulation, the problem of nanofocusing poses an interesting challenge. Transport of energy begins at a macroscopic scale, where electrodynamics applies, and it then proceeds to length scales spanning only a few atoms, a regime where quantum and nonlocal effects govern the propagation of electromagnetic waves.

Previous descriptions of nanofocusing cones were based on local solutions of Maxwell's equations, which restricted the validity of the solutions to distances many tens of nanometers away from the sharp end of metallic tips. In my work, I have developed a solution which takes into account the effects of nonlocality, making it valid even for sub-nanometer length scale. This makes it suitable for the investigation of surface roughness effects. Interestingly, we found that effects of nonlocality mitigate this adverse influence of surface roughness, restoring the amplitude of the hot spot to a larger value than would be expected from local solutions of Maxwell's equations. This insights into the effects of nonlocality on electromagnetic surface waves are not limited to metallic tips, but apply equally to other devices which rely on the propagation of electromagnetic energy on metallic surfaces.

The publication which forms the subject of this highlight— **Wiener, A.**; Fernández-Domínguez, A. I.; Horsfield, A. P.; Pendry, J. B.; Maier, S.A. Nano Letters (2012), **12** (6), pp 3308–3314.



Research Highlight:
Towards a Multiscale Model for Polymer Membranes

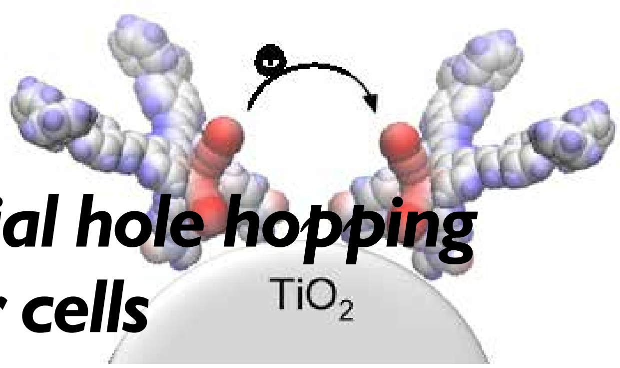
***Richard Broadbent** (Cohort 1) won the 2011 Materials Design Early Stage Graduate Research Prize for showing us that good physics can actually have real life applications. Here he explains his work:*

For centuries people have been separating materials into different phases. One highly desirable example is the separation of drinking water from sea water. This can be achieved through evaporation; however, it was demonstrated in the 1950's at UCLA that it was possible through the use of membranes. This process was initially highly inefficient but modern day plants can produce 100,000–300,000m^3 a day of purified water. For comparison, a large oil refinery can process between 50,000 and 100,000m^3 a day of crude oil by means of fractional distillation.

My research focuses on building a computer model for the manufacturing process used to make polymer membranes for filtering molecules out of organic solvents. These membranes are becoming widely used; however, at present their design is a matter of trial and error which can be very costly. A better theoretical understanding of these membranes could lead to more efficient designs. Unfortunately the manufacturing process takes place on a timescale of seconds and a length scale of micrometres, whilst the interactions that dominate the formation take place on a femtosecond timescale and less than a single nanometre in length.

Conventional approaches cannot study such phenomena, so we designed a multiscale approach taking information from the quantum scale and passing it through atomistic simulation methods into a coarse grained molecular level. This allows us to study how the pores which allow filtration are formed as well as looking at aspects such as connectivity to understand how the network of unconnected polymer strands work as a filter. This may lead to new membranes which could significantly reduce both the cost and energy consumption of their use in pharmaceutical and chemical manufacturing processes.

Research Highlight: *Modelling of interfacial hole hopping in dye-sensitised solar cells*



Valerie Vassier *(Cohort 2) introduces her research, which has been selected for special mention by CDT Director Peter Haynes:*

I am of the kind obsessed with nature and wildlife: nothing makes me happier than the sight of an animal. It is a great shame then that our current way of living seems to be leading to the demise of the environment. Can we do something to fight back? I believe so—being French, I have an ego that makes me sure I can change the world for the better!

However, I won't lie—finding a niche in the fight against climate change is anything but trivial. Luckily for me, I settled on a PhD project that nicely combines my primary motivations with my eagerness for rigour and logic: simulation of charge transport in solar cells. My three supervisors, Jenny Nelson, Piers Barnes and James Kirkpatrick, have complementary areas of expertise and help me by building my very own skill set.

The systems I work on are Dye Sensitised Solar Cells (DSSC) in which the light absorber is a molecule: the dye. The absorption of a photon by the dye results in an exciton which eventually splits up into electron and hole. Since the efficiency of a solar cell relies on the current it produces, efficient transport of these charges is highly important for good devices.

I want to simulate the movement of holes from one dye to another. Numerical work is crucial for a systematic study where the effect of each possible parameter can be independently quantified. Indeed, in addition to lacking accuracy, experimental data on the nanoscale is not accessible.

Starting with the smallest length scale—the characterization of one hole hop between two dyes—I calculated the influence of the chemical structure of the dyes, their relative orientation and the effect on hole hopping rate. The latter has led to a publication ***"Influence of polar medium on the reorganization energy of charge transfer between dyes in a dye sensitized film"*** in the Journal of Chemical Physics.

Of course, I haven't stopped there: I am now trying to scale up my results, investigating the likelihood of a succession of hops. This requires accounting for the true configuration of the dyes as not only do they sit on the surface of nanoparticles but they are also randomly arranged (configurational disorder). By gradually progressing from the nano to the microscopic scale, we hope to acquire a solid computational tool to predict and therefore control the kinetics of charge transport.

'A summer school to find them, a summer school to bring them all and in the TSM bind them'

Every year the TSM-CDT runs a summer school for undergraduates - with good reason.

'*There are three things extremely hard: steel, a diamond, and to know one's self*' (Benjamin Franklin).

Many students of the physical sciences, particularly at the theoretical end of the spectrum, are attracted by the challenge of using mathematics to describe and predict the way the world works. Many engineering students are motivated by a desire to apply their skills to find technological solutions to contemporary societal problems. Students in TSM enjoy both of these incentives, but it is often difficult to persuade talented undergraduate students to move into the multidisciplinary field of materials that is often misunderstood. How can a budding theoretical physicist be convinced that polymers can be as intellectually challenging as string theory? What does it take for a promising mechanical engineer to switch from design problems to the simulation of complex fluids?

From 3rd-6th July the TSM-CDT once again hosted the annual London Summer School on Theoretical Materials Science. Under the leadership of Dr Carla Molteni from King's College London, the aim of the school was to provide students with a taste of cross-disciplinary life in the TSM-CDT. Each of the four days focused on a different length-scale: fluid dynamics with Dr Berend van Wachem from Imperial, molecular dynamics with Prof Ian Ford from UCL, electronic structure quantum-mechanical calculations with Dr Carla Molteni and kinetic Monte Carlo with Prof Lev Kantorovich from King's College London. Morning lectures provided an introduction to the relevant theory, leading in to hands-on computational classes in the afternoon. Feedback from the undergraduates who participated in the school was overwhelmingly positive, some expressing a keen interest in finding out more about TSM and the CDT. One wrote that "*the school was brilliant at giving a flavour of what life in a CDT is like.*" That is exactly what we hoped for.

Chairman Sutton and Dr Dini win the Rector's Favour

***Prof Adrian Sutton** and **Dr Daniele Dini** (Mentor to Cohort 3) win awards in recognition for their outstanding contributions in the field of excellence! **Beñat Gurrutxaga-Lerma** (Cohort 2) congratulates his supervisors:*

Max Weber advised all those wishing to begin a scientific academic career that they should only do so if they firmly believed they could live without recognition despite their qualities or, worse, by having to bow to that granted to less meritorious recipients. It was perhaps with the intention of countering that pessimistic observation that the Imperial College Rector has come to recognise the outstanding contributions members of staff may make *beyond* their research with the Rector's Awards for Excellence. And if the awards were to be judged by this year's recipients, we could be certain that not only have they not been awarded in vain but, quite the opposite, they have never been more deserved: this year's recipients were Prof Adrian Sutton and Dr Daniele Dini, both academics in our CDT.

Thus, our founding father Prof Adrian Sutton FRS has been announced the recipient of two of these awards: the Rector's Medal for Outstanding Innovation in Teaching, and one of the Rector's Awards for Excellence in Teaching. Both are awarded for outstanding contributions in teaching, which in the case of Prof Sutton reflects his efforts both in setting up the CDT and in his latest endeavour, the pan-academic Imperial Horizons course for undergraduates. In this, he tries to offer scientists-to-be a scope broader than that of mere science by introducing them to some of the social and economic impacts their work might have. Prof Julia Buckingham (Pro Rector for Education and Academic Affairs) commented that "*it is a very fitting tribute for all Prof Sutton has done both for the CDTs and Horizons, both of which have been hugely beneficial to our students and have had a huge influence on the thinking of how we should be educating our students.*"

As for Dr Daniele Dini, Mentor to Cohort 3, he was the winner of one of the Rector's Award for Excellence in Research Supervision and, on top of that, the Rector's Medal for Excellence in Research Supervision. These awards celebrate staff that are considered to show "*exemplary activity in inspiring and supporting students throughout their studies.*" Those who are lucky enough to have Daniele as a supervisor know that few people could deserve this award more than he does. It is a well-deserved award, and we wish to congratulate Daniele for it.

Multi-scale Mastery

*The prestigious Materials Design Late Stage Graduate Research Prize is awarded to **Joe Fallon** (Cohort 1). Following a version control nightmare, one academic and three CDT students report.*

The prestigious Materials Design Late Stage Graduate Research Prize has been awarded to Joe Fallon. This prize of £600 is kindly sponsored by Materials Design to acknowledge the TSM student who has demonstrated the most significant progress during their second year of PhD study. Recognising the strength of all candidates, Prof. Peter Haynes commented on the difficulty of allocating this award, but remarked that "*the committee was particularly impressed by Joe's achievements in successfully spanning length- and time-scales in a very challenging system.*"

Joe's research focuses on ferroelectric materials, widely used in modern electronics. The industrial drive towards ever smaller ferroelectric devices has created a need to understand their properties on the atomistic scale, and Joe's aim is to simulate ferroelectrics at the mesoscopic length scale while retaining the accuracy of full atomistic quantum-mechanical simulations. To this end he has created a classical force-field for the ferroelectric barium titanate (BTO) which accurately reproduces many properties as calculated via density-functional theory (DFT). Joe has further used DFT to parameterise an atomistic force-field for BTO using force matching methods. According to Dr Arash Mostofi (one of Joe's supervisors) "*the force-matching approach is rather challenging in this case*", referring to the complexity of the true potential energy surface, and the subtle sensitivity of ferroelectricity to volume. Despite these challenges, Joe has succeeded in making a force field that reproduces the DFT structures and phonon bands to a very high level of accuracy and good agreement with the existing literature.

"The multi-scale aspects of my project are the most challenging," Joe remarked, echoing the thoughts expressed by both Peter Haynes and Arash Mostofi on the complexity of performing multi-scale work. *"I spent a long time on DFT calculations and then had to jump suddenly to molecular dynamics simulations. In the CDT community I am able to chat to fellow students who have already been using the new techniques I need to learn from their advice and experience."*

Having an accurate atomistic force-field for BTO will enable Joe to study fundamental questions regarding this material, for example, the precise nature of the paraelectric–ferroelectric transition, surface and domain boundary structures, and how the Curie temperature varies with sample thickness. The CDT wishes him the best of luck with his future research.

Hermes 2012

The International Materials Modelling Summer School

*Students **Jassel Majevadia** and **Aeneas Wiener** (Cohort 1) on their summer school-turned-global phenomenon,* **Hermes 2012**

During the opening weekend of the London 2012 Olympic games, 20 graduate students from across the London universities teamed up to orchestrate Hermes 2012, London's first summer school on Materials Modelling and Science Communication. The tag line of Hermes was to marry good science and good science communication, and to bring it to students from around the world. While the event was primarily aimed at further encouraging cross-disciplinary thinking within materials science, the team was able to use it as an opportunity to build a global network of students who, it is hoped, will continue to collaborate in the future on the interdisciplinary challenges facing materials science. With the impact and applicability of research becoming paramount, the last aim of Hermes 2012 was to enable these excellent researchers to communicate their research to the wider world using a variety of media.

Hermes was a student-led initiative, developed and co-chaired by Jassel Majevadia and Aeneas Wiener. Other members of the organising team stemmed from the TSM CDT, Queen Mary's University, King's College London, and UCL. In collaboration with Imperial College's Science Communication department and a team from the BBC, the committee developed a series of masterclasses in modelling methods and a workshop on communicating science via video media, meeting once a week througout the preceding year in a trendy coffee shop in Soho, where ideas were discussed and then brought to life.

Based at Cumberland Lodge in Windsor Great Park, the global network of participants experienced a sunny weekend in the company of four of the world's finest materials scientists. Professor Vaclav Vitek of the University of Pennsylvania, one of the world's authorities on fracture mechanics, delivered a talk on understanding such a macroscopic phenomenon at the atomic level. Developer of the commercial ab initio modelling package CASTEP, Professor Chris Pickard of UCL gave a gripping talk on the nature of truly condensed matter, describing the pressures experienced at the centre of Jupiter and the ability of simulation techniques to predict structures in these high-pressure environments. The subtle distinction between strength and toughness in a material were conveyed by Professor Helena van Swygenhoven of the Paul Scherrer Institute, who emphasized the need to combine good theory and good experimental techniques to continue pushing the frontiers of materials science. Finally, Professor Craig Carter from MIT, debuted his talk on the beauty of calculus within the science of phase transformations and as art, using phase field and finite element simulations performed in real time. He then concluded his master class with a display of some of his most recent scientific works of art, which are currently on display at the Smithsonian, New York's Museum of Modern Art and at Paris' Pompidou Centre.

In addition to the four invited speakers, there were 51 participants of the summer school. They originated from countries as distant in geography and in culture as Argentina, Brazil, Singapore, South Africa, Nigeria, Kenya, India and all across Europe. This global nature of the event was demanded by the organising team, who worked hard to obtain sponsorship in the region of £10,000 from the Royal Society of Chemistry and Unilever. This helped fund the registration and travel of six scholarship winners from developing nations.

True to the spirit of the Olympics and friendly competition, the cohort of participants were split into eight teams who were then given a mere 24 hours to storyboard, film and edit a short film explaining a materials science concept from the masterclass lectures to a general audience. The videos can be found on the Hermes Academy Youtube page. The winning team received an iPod Touch (generously provided by the London Centre for Nanotechnology) as a prize, which should enable them to continue to create good scientific media in their home institutions!

The Mpemba Effect

In the run up to Hermes 2012 the organising team launched the £1000 RSC-Hermes Challenge: Explain the Mpemba effect, or "Why does hot water freeze faster than cold water?" The aim of the challenge was to obtain media exposure for the event, and to explore new ways for scientists to interact with the general public, inspiring scientific and creative thinking amongst the general public. Following the competition's launch on June 26, the challenge has attracted over 20,000 submissions from amateur scientists over the world. The Hermes server nearly crashed when thousands of participants wrote in with their attempts to answer this seemingly simple question, which has continued to baffle scientists since the days of Aristotle.

The viral success of the challenge brought Hermes 2012 a great deal of interest from the press, including BBC Radio 4's World at One show and Channel 4 News. In addition, the story has been covered by the online and print editions of the Guardian, the Daily Mail, and the Telegraph.

Visiting Professors
Richard Martin

Hosted **27th June–1st July 2011**, *Masterclass organiser* ***Tom Poole*** *(Cohort 2) reports on the visit by an Electronic Structure giant:*

Professor Richard Martin received his PhD in physics from the University of Chicago in 1969. After a couple of years spent on the technical staff of Bell Labs he was appointed as chief scientist at the Xerox Palo Alto Research Center and as a consulting professor at Stanford University, then assuming a position as professor in the physics faculty at the University of Illinois in 1988. Professor Martin is a recipient of the Alexander von Humboldt Senior Scientist Award, is a Fellow of the American Physical Society (APS) and the American Association for the Advancement of Science. He has also served on several editorial boards of the APS including Physical Review, Physical Review Letters and Reviews of Modern Physics where he was associate editor for condensed matter theory.

Professor Martin's work can be broadly classified into theoretical contributions to our physical and formal understanding of the electronic properties of solids and technical contributions to computational methods for materials. His collaboration with Prof David Ceperley–based at the University of Illinois and the National Center for Supercomputing Applications–focuses on the development of accurate ab initio calculations of the properties of condensed matter. A particular goal of the work is to enable the calculation of macro-scale material properties via the application of several different computational methods, beginning from many-body quantum Monte Carlo simulations and density functional calculations. Other research interests include the metallisation of hydrogen at high pressure, electronic structure at finite temperatures and in strong magnetic fields, and the study of doped fullerenes using a new method for Monte Carlo simulations of interacting electrons.

The CDT received a series of lectures from Professor Martin focused on condensed matter theory. Topics covered independent particle approximations, excited states and time-dependent density functional theory, many-body methods, and the calculation of mechanical and electro-mechanical properties of materials. Students also got the opportunity to interact with Professor Martin and discuss their research in private meetings throughout his time at Imperial College.

A sequel to Prof Martin's textbook Electronic Structure: Basic Theory and Practical Methods (CUP, 2004), a stalwart component of any practioner's library, is soon to be published. Written in collaboration with Prof David Ceperley, its focus will be on the problem of 'strong correlation', and the quantum Monte Carlo techniques employed in its study.

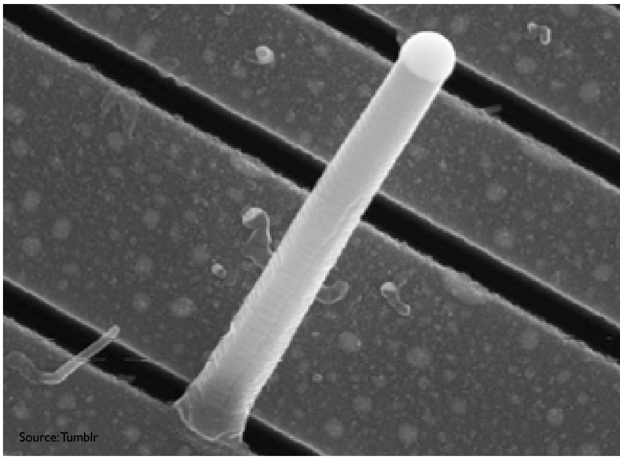
Visiting Professors
Jerry Tersoff

The TSM–CDT hosted IBM's very own PRL-writing machine between the **19th July–4th August 2011.** ***Richard Broadbent*** *(Cohort 1) who organised the visit, gives this report:*


Source: IBM

Dr Jerry Tersoff is one of the most highly respected scientists in the world. Shortly after getting his PhD from Berkeley, he entered the IBM Thomas J. Watson Research Center laboratories, where he has grown to become a true giant of materials research, with over 28,000 citations and an impact h-index of 72. During his 28 years at IBM, his research interests have extended from the atomic scale, where he invented the new form of potentials known as Bond Order Potentials, to the continuum scale, where his recent work modelling nanowire growth has led to new discoveries in the field. His research into both the electronic and structural properties of semiconductors has helped IBM maintain its position as a key player in semiconductor research. The main characteristic of his research is perhaps the use of simple models to describe complex behaviour.

In the summer of 2011 Jerry Tersoff visited Imperial for two weeks to give a highlight seminar to the Thomas Young Centre and a two part master class on modelling to the cohorts of the TSM CDT. The focus of these masterclasses was on how to approach the modelling of the growth of semiconductor nanowires using simple thermodynamic concepts instead of atomistic brute-force simulations.


Source: Tumblr

Whilst he was visiting the majority of TSM students took the opportunity to meet with him in a one-on-one setting and discuss their research. Apart from offering the students a unique chance of meeting one of the top researchers worldwide, these meetings were often very productive, to the point that some of our students fundamentally altered their research approaches based on his advice.

Visiting Professors
Vaclav Vitek


Source: University of Pennsylvania

Hosted **30th July—17th August 2012**. ***David Trevelyan*** *(Cohort 2) describes the visit of the (unofficial) Grandfather of the TSM CDT*

The TSM CDT was delighted to welcome Professor Vaclav Vitek to Imperial College this August. A true pioneer, Professor Vitek played a pivotal role in laying the groundwork for what was once the young field of computational materials science, but which has since grown to be one of the most important branches of science and engineering. Professor Vitek graduated in his native Czech Republic in the 1960s. After spending a few years in Oxford, in 1978 he moved to the University of Pennsylvania as a full professor, where he remains to date.

The thrust of Professor Vitek's research is multiscale modelling of deformation and fracture behaviour of materials that links electronic, atomic, nano, and macroscopic scales. He works principally on the atomic level, which includes development of interatomic potentials that reflect both metallic and covalent aspects of bonding, as well as properties such as ferromagnetism. This modelling involves atomistic studies of dislocations and their glide modes, structure and properties of interfaces, and interactions of these extended defects with other crystal defects. As such, Prof Vitek's work has been the real inspiration behind the establishment of our CDT, and if not its founding father—a title one of his PhD students, Prof Adrian Sutton FRS deserves—he could at least be considered its grandfather.

Professor Vitek delivered a set of three workshops on a variety of computational materials science techniques, in addition to two seminars on his recent work in multiscale modelling of plastic deformation and non-planar dislocation cores as part of the Thomas Young Centre's 'Highlight' series. He insisted that multiscale analysis is seldom about transferring numbers from one scale to another, but using the qualitative descriptions of the physics in one scale on another.

Lessons in Success

TSM's Masterclass from ex BP VP, Vivienne Cox


Source: Pearson

As part of the prestigious TSM Masterclass series, **Vivienne Cox,** *former Vice President of BP, visited the CDT to share stories from her illustrious career.* ***Joe Fallon*** *(Cohort 1), mindful of the Chatham House Rules, nonetheless manages this report:*

On the 15th November a Masterclass for TSM students was led by Vivienne Cox. Vivienne is currently a non-executive director of several different organisations including Rio Tinto, Climate Change Capital and the Department of International Development.

Vivienne has a scientific background: she studied chemistry. Upon graduating, she entered British Petroleum, where she began her career in a technical position then to swiftly move forward to a more managerial one. After gaining an MBA from INSEAD, Fontainebleau sponsored by BP, she lead the team that set up BP's commodity derivatives group, and then went on to re-organise the supply and trade organisations within BP. She worked her way up through BP to become CEO of BP Alternative Energy, thus bringing together (and, to a big extent, helping develop) BP's alternative energy operations. As an executive vice-president, she became the most senior woman in BP of her time, gaining invaluable business expertise along the way. Vivienne left BP in 2009, and has since devoted herself to her family and non-executive roles.

At the Masterclass a lively discussion was held, covering areas such as the working environment at different types of companies and different viewpoints on the corporate world. Some surprising revelations were made. However, following the Chatham House Rules, these shall not be disclosed in this article. The event gave a real insight into the world of business and encouraged us to consider whether we would like to work in that sector after our PhDs.


Source: Wikimedia Commons

Sir Bill Wakeham Masterclass

Years after the 'Wakeham Review' comes the 'Wakeham Interview'

Sir Bill Wakeham's lifetime of expertise in the intricacies of the UK's university and research systems is shared in an exclusive interview with the TSM-CDT's ***Nina Kearsey*** *and* ***Beñat Gurrutxaga–Lerma*** *(Cohort 2):*

Source: University of Southampton

Q: *Are Universities like dethroned monarchs–always begging for more money?*
W: Ha! Well, I think there is an arrogance about universities–which is perhaps what you mean by '*dethroned monarch*'–that leads them sometimes to believe that there is an entitlement to being funded, as opposed to proven merits or demonstrable needs. But I do not think it is institutions as such that behave that way: it is the academic body that does it. Of course, vice-chancellors by and large are drawn from the academic body, so you see that kind of behaviour in them too: not quite begging for money, but more a "*we deserve it*".

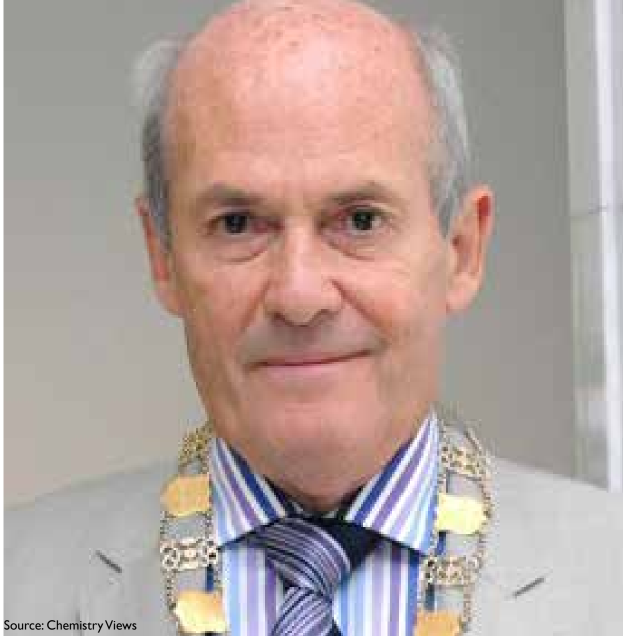
Q: *So if funding resources were plentiful, do you think academia would try to produce something useful to society, as it often claims it does?*
W: I think academia, understood as individuals that form it, would fractionate in two groups: there are many people whose entire intent is for what they do to be of benefit to society; whereas there are other individuals who behave solely in their own interest, no matter how remote from practical interest. It might be just for the lack of resources, but I would say that that balance has shifted now more towards the number of those who would make something for society. Anyway, there are a few of the others left.

Q: *Do you think then that universities as a body should be more geared towards producing research that is going to enrich society?*
W: Yes. That should be the purpose of all universities; and many of them will have something like that at the heart of their mission statement or charter. And I think it is happening more, the reason for which being that the big problems that the world faces nowadays impact more or less directly on society in a way they perhaps did not some time ago: there is now more understanding of that interaction between society and science than there was before in the scientific community. On the other hand, you cannot always just do what society needs, because "driven by problems" research will not necessarily come up with a breakthrough.

Q: *Would it then be better to let universities let conduct blue-skies research, and let other institutions and private enterprises apply this newly acquired knowledge to something of social relevance?*
W: The short answer to that question is no. Universities should be conducting a complete portfolio; perhaps different universities on a different aspect of that portfolio or with different concentrations of resources. Universities should not only be conducting basic research but, at the same time, stimulating those outcomes of this research. I will refer to the notion of 'exploitation' not in the sense of the university to make a profit: it is to make the money to flow back into it. My proudest example of this exploitation happened when I was in Southampton, where we had one company that came out of the oceanography centre: we formed the company, sold some of the shares and invested the money in an undergraduate facility–a ship, as it happened, for undergraduates to use for research and their projects. And that was the first time I achieved what I consider the virtuous circle: getting funding back into teaching.

Q: *So is the direct participation of private companies in academic research desirable?*
W: Under the right conditions yes; and I think the complexity is around the right conditions. Some time

ago universities were obsessed with holding the intellectual property of their research; all they wanted was to control and hold it, but little more: they would not invest and get something out of it, because that was '*too risky*'. I think that that attitude is over, because universities finally understood that owning it all is not the point: it is getting the value out of it. Now, private companies allow the exploitation; they are the vehicle for getting it out into the market. What you must be careful of is having the research output vetoed by a company. There are sophistications to the way the business world operates the university has to understand.


Source: Chemistry Views

***Q:** And what about government funding? It would seem that the idea of pumping money into concrete research areas by the government is actually quite a socialist idea, which makes the readiness with which it has been adopted as a common practise for example in the US quite remarkable. Do you agree?*

W: Ha! Rather than 'socialist', I might have said 'totalitarian', which could be right-wing as well: it is essentially a state-run operation. In this country, unusually, government science funding follows the so-called *Haldane Principle*; government decides how much it will spend in science, but it has no influence whatsoever (until recently) on what project will be funded. None. That decision is taken entirely within the academic community. And that principle of separation between deciding the amount of money spent from what project gets funded separates the state from what gets done; it does not change the notion of the amount of what gets done–the total. Now there is a problem associated with that, which is that government could find it very difficult to intervene, to be strategic. So if it has an industrial policy, how does it make sure that universities and the research councils fund things that match this industrial policy? Quite a challenge! The government invented the so-called TSB (Technology Strategy Board) which funds problem-driven research at a different technology readiness level–closer to the market needs–and has tools such as the research assessments (RAE) to concentrate resources.

***Q:** Related to that, and the allocation of research grants: do you think that trends in research grants dictate what academics can do? For example, in Materials we know that if we mention solar cells or green energy, we are more likely to get grants. So, in this sense, are we doing the research that we want to do, or are these trends determining the academic agenda for us?*

W: Going back to my point about strategy for the country: if the government–and other countries' governments do this better than we do–has an industrial strategy that decides to concentrate in, say, solar cells, then, to speed up your industrial strategy, you need to find a way to concentrate the research on that area. That does not prescribe what you finally end up doing in solar energy–you have the blue-sky prospectus that determines that–but it does mean you want it focused around that area. The typical academic response to that is "*I need to put the word 'solar cell' into a proposal even if I'm actually interested in farm animals*". You can obviously only stretch that so far. But is that bad for the strategy, that somebody is adjusting their agenda to look as though they were doing solar cell research? I do not think so. It does not totally distort the agenda; it has a tendency to, but that is probably reasonable.

***Q:** Of course, especially in the present context of economic crisis, state funding and resources are limited, so one would think that focusing is inevitable...*

W: Indeed, I think that the UK can no longer afford to do everything in science: it is just too expensive and we are not a big country. I actually believe most countries cannot; not even the US can afford to do absolutely everything! So you need to choose. Once that happens, there is an inevitable focusing, and people will need to be flexible enough to move their activity closer to what you want–not on top of what you want, but closer to it. And that seems to me a price to pay if you want to continue to work, and to live in this country. If you want complete freedom, I do not think there is a country that would allow you to research with unfettered resources.

Current Students and Research Projects

Cohort 1

Richard Broadbent—*A Multi-scale Model for Deformation of Polymers*

Prof Adrian Sutton (Physics), **Dr Arash Mostofi** (Materials/Physics), **Prof Andrew Livingston** (Chem. Eng.), **Dr James Spencer** (Materials)

David Edmunds—*Course Grained Classical and Quantum Molecular Dynamics*
Prof Matthew Foulkes (Physics), **Prof Dimitri Vvedensky** (Physics), **Dr Paul Tangney** (Materials/Physics)

Joseph Fallon—*Multi-scale Theory and Simulation of Nanoscale Ferroelectric Materials*
Dr Arash Mostofi (Materials/Physics), **Dr Paul Tangney** (Materials/ Physics)

Robert Horton—*The thermodynamics of charged defects in ionic crystals*

Prof Mike Finnis (Physics/Materials), **Prof George Jackson** (Chem. Eng), **Prof Amparo Galindo** (Chem.Eng.)

Jassel Majevadia—*Multiscale modelling of precipitates in zircaloy cladding*
Dr Daniel Balint (Mech.Eng.), **Dr Mark Wenman** (Materials), **Prof Adrian Sutton** (Physics)

Aeneas Wiener—*Theoretical Investigation of Superfocusing*

Dr Andrew Horsfield (Materials), **Prof Stefan Maier** (Physics)

Cohort 2

Anthony Lim—*What excited electrons do*

Prof Matthew Foulkes (Physics), **Dr Andrew Horsfield** (Materials), **Dr Daniel Mason** (Physics)

Jawad Alsaei—*Theory and simulation of the dielectric properties of functional oxide thin films*
Dr Arash Mostofi (Materials/Physics), **Dr Paul Tangney** (Materials/Physics), **Prof Neil Alford** (Materials)

Niccolo Corsini—*Pressure-induced structural transformations in nanomaterials*
Prof Peter Haynes (Materials/Physics), **Dr Carla Molteni** (KCL Physics), **Dr Nicholas Hine** (Materials)

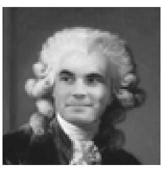
Beñat Gurrutxaga–Lerma—*Theory and simulation of elastoplasticity at very high strain rates*
Dr Daniel Balint (Mech.Eng.), **Dr Daniele Dini** (Mech.Eng.), **Dr Daniel Eakins** (Physics), **Prof Adrian Sutton** (Physics)

Mohamed Ibrahim—*Mechanical properties and decohesion laws of crystalline Titania-based smart coatings*
Dr Daniele Dini (Mech.Eng.), **Prof Alessandro De Vita** (KCL Physics), **Prof Nic Harrison** (Chemistry)

Thomas Poole—*Force Fields for Carbon Nanostructures via Algorithmic Differentiation*
Prof Matthew Foulkes (Physics), **Dr James Spencer** (Materials/Physics), **Prof Peter Haynes** (Materials/Physics)

Fabian Renn—*Investigating the spatio-temporal dynamics of amplification and gain in nano-plasmonic metamaterials at different lengthscales*
Prof Ortwin Hess (Physics), **Dr Andrew Horsfield** (Materials), **Dr Rupert Oulton** (Physics)

Thomas Swinburne—*Fluctuating dynamics of nanoscale defects and dislocations in nuclear materials*
Prof Adrian Sutton (Physics), **Dr Sergei Dudarev** (Culham Centre for Fusion Energy), **Dr Steve Fitzgerald** (Culham Centre for Fusion Energy)



David Trevelyan—*Multiscale simulations of instabilities in complex non-Newtonian fluids*
Dr Tamer Zaki (Mech.Eng.), **Dr Daniele Dini** (Mech.Eng.), **Dr Fernando Bresme** (Chemistry)

Joshua Tsang—*Interfacial free energy of solid-melt interfaces in light metals and alloys*
Prof Mike Finnis (Physics/Materials), **Prof Alessandro De Vita** (KCL Physics), **Prof Peter D Lee** (Manchester Materials)

Valerie Vaissier—*Modelling of interfacial hole hopping in solid state dye sensitised solar cells*
Prof Jenny Nelson (Physics), **Dr Piers Barnes** (Chemistry),
Dr James Kirkpatrick (Oxford Mathematics)

Tim Zuehlsdorff—*Theory and simulation of metal/semiconductor nano-particle interfaces for solar energy storage*
Prof Peter Haynes (Materials/Physics), **Dr James Spencer** (Materials),
Prof Nic Harrison (Chemistry), **Prof Jason Riley** (Materials)

Cohort 3

Vincent Chen—*Simulation of the solid/liquid interface for Chalcopyrite leaching*

Dr Patricia Hunt (Chemistry), **Prof Nic Harrison** (Chemistry)

Marc Coury—*Evolution of non-collinear magnetism in hot iron*

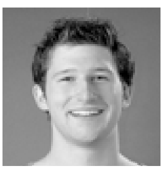
Dr Andrew Horsfield (Materials)**, Prof Matthew Foulkes** (Physics)

Thomas Edwards—*A Multiscale Study of Extremely Thin Absorber solar cells*

Dr Andrew Horsfield (Materials), **Prof Nic Harrison** (Chemistry)

Ali Hammad—*A new model of mechanical properties of aligned polymers*

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)

Mohammed Khawaja— *A hierarchical computational approach to interfacial dynamics*
Dr Tamer Zaki (Mech.Eng.), **Dr Pedro Baiz Villafranca**(Aeronautics),
Dr Janet Wong (Mech.Eng.)

Karlis Kramens— *Multiscale investigation of failure in bonded diamond aggregate*
Dr Daniele Dini (Mech.Eng.), **Dr Daniel Balint** (Mech.Eng.), **Prof Adrian Sutton** (Physics), **Dr Serdar Ozbayraktar** (Element 6)

Gabriel Lau—*Droplets: from molecular nanoclusters to the atmospheric aerosols*
Prof George Jackson (Chem.Eng.), **Dr Patricia Hunt** (Chemistry), **Prof Ian Ford** (UCL Physics)

Tairan Liu—*Radiation damage mediated processes in nuclear fuels*

Prof Robin Grimes (Materials), **Dr Mark Wenman** (Materials)

Joel Posthuma de Boer—*Epitaxial Graphene*

Prof Lev Kantorovich (KCL Physics), **Prof Dimitri Vvedensky** (Phsycis)**, 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 Selassie Dorvlo** (JM)**, Dr Michele Marigo** (JM)

Christopher Rochester—*Dynamics of ionic liquids in confinement and the performance of ionic liquid based electroactuators*
Prof Alexei Kornyshev (Chemistry), **Prof Gunnar Pruessner** (Mathematics)

Cohort 4 – a warm welcome!

Max Boleininger, Stephen Burrows, Gil–Arnaud Coche, Jacob Craigie, Andrea Greco, Chiara Liverani, Thomas Moran, Adam Ready, Michael Ridley, Mahdieh Tajabadi Ebrahimi, Michael Stumpf, Robert Wilson

Alumni News

Frank Bruijnsters (Cohort 2), after having passed the MSc in TSM with distinction, is now pursuing a PhD at Radboud University of Nijmegen.

Members of the Advisory Board

External Advisors

Prof W Craig Carter – MIT, USA
Dr Sergei Dudarev – EURATOM Fusion, UK
Dr Claire Hinchliffe – Sheffield-Manchester CDT, UK
Dr John Casci – Johnson-Matthey, UK
Prof Paul Madden FRS – Oxford, UK
Prof Paul O'Brien – University of Manchester
Ms Alexandra Peden – EPSRC
Prof Danny Segal – CQD-CDT, Imperial College, London
Dr Mike Steeden – DSTL
Prof Helena Van Swygenhoeven – Paul-Scherrer Institute & EPFL, Switzerland
Prof Dominic Tildesley – Director of CECAM

TSM CDT Members

Prof Peter Haynes – Director
Prof Adrian Sutton FRS – Chairman
Dr Arash Mostofi – Deputy Director/Cohort Mentor: cohort 1&4
Dr Patricia Hunt – Cohort Mentor: cohort 2
Dr Daniele Dini – Cohort Mentor: cohort 3
Dr Simon Foster – Outreach Officer
Mr Julian Walsh – External Relations Director
Ms Lilian Wanjohi – Board Secretary

List of Staff
Imperial College London

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Dr Michael Bearpark *(Chemistry)*
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Dr Maria Charalambides *(Mechanical Engineering)*
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Prof Matthew Foulkes *(Physics)*
Prof Amparo Galindo *(Chemical Engineering)*
Dr Finn Giuliani *(Materials)*
Dr Chris Gourlay *(Materials)*
Prof Robin Grimes *(Materials)*
Prof Yannis Hardalupas *(Mechanical Engineering)*
Prof Nic Harrison *(Chemistry)*
Dr Andrew Haslam *(Chemical Engineering)*
Prof Peter Haynes *(Materials and Physics) – Director*
Dr Jerry Heng *(Chemical Engineering)*
Prof Ortwin Hess *(Physics)*
Dr Sandrine Heutz *(Materials)*
Prof David Heyes *(Mechanical Engineering)*
Dr Nicholas Hine *(Materials and Physics)*
Dr Andrew Horsfield *(Materials)*
Dr Patricia Hunt *(Chemistry) – Second Cohort Mentor*
Prof George Jackson *(Chemical Engineering)*
Prof Lorenzo Iannucci *(Aeronautics)*
Prof John Kilner *(Materials)*

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Prof Norbert Klein *(Materials)*
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Dr Rongshan Qin *(Materials)*
Prof Nick Quirke *(Chemistry)*
Prof Jason Riley *(Materials)*
Dr Ferdinando Rodriguez y Baena *(Mechanical Engineering)*
Prof Mary Ryan *(Materials)*
Prof John Seddon *(Chemistry)*
Prof Nilay Shah *(Chemical Engineering)*
Prof Spencer Sherwin *(Aeronautics)*
Dr James Spencer *(Materials and Physics)*
Prof Adrian Sutton FRS *(Physics) – Chairman*
Dr Paul Tangney *(Materials and Physics)*
Dr Alex Thom *(Chemistry)*
Dr Berend van Wachem *(Mechanical Engineering)*
Prof Dimitri Vvedensky *(Physics) – Admissions Tutor*
Prof Tom Welton *(Chemistry) – Research Board*
Dr Mark Wenman *(Materials)*
Prof Gordon Williams *(Mechanical Engineering)*
Dr James Wilton-Ely *(Chemistry)*
Dr Janet Wong *(Mechanical Engineering)*
Dr Tamer Zaki *(Mechanical Engineering)*
Prof Robert Zimmerman *(Earth Science & Engineering)*

Academics from Other Institutions

The following academics have proposed research projects and/or are supervising students in the TSM-CDT:

Prof Alessandro De Vita *(King's College London)*
Prof Andrew Fisher *(University College London)*
Prof Ian Ford *(University College London)*
Prof Daan Frenkel ForMemRS *(University of Cambridge)*
Prof Mike Gillan *(University College London)*
Prof Lev Kantorovich *(King's College London)*
Dr James Kirkpatrick *(University of Oxford)*
Prof Peter Lee *(University of Manchester)*
Dr Chris Lorenz *(King's College London)*
Prof Angelos Michaelides *(University College London)*
Dr Carla Molteni *(King's College London)*
Prof Alex Shluger *(University College London)*

External Collaborators and Partners

Those who are collaborating on research projects or have contributed to the delivery of transferable skills courses:

Dr Mike Butler *(Unilever)*
Dr Ann Canham
Dr David Curry *(Baker Hughes)*
Dr Selassie Dorvlo *(Johnson Matthey)*
Dr Sergei Dudarev *(Culham Centre for Fusion Energy)*
Ms Lucy Esdaile *(Rio Tinto)*
Mr Mike Fish *(Element Six)*
Dr Steve Fitzgerald *(Culham Centre for Fusion Energy)*
Dr John Freeland *(Argonne National Laboratory)*
Dr Nick Green *(The Royal Society)*
Mr Donald Hockmuth *(Materials Design)*
Dr Julius Jellinek *(Argonne National Laboratory)*
Mr Alok Jha *(The Guardian)*
Mr Dan Johns *(Bloodhound SSC)*
Dr Anatole von Lilienfeld *(Argonne National Laboratory)*

Dr Pui-Wai (Leo) Ma *(Culham Centre for Fusion Energy)*
Dr Michele Marigo *(Johnson Matthey)*
Dr Duncan McInnes *(Bank of America Merrill Lynch)*
Dr Serdar Ozbayraktar *(Element Six)*
Dr Ruth Pachter *(US Air Force Research Laboratory)*
Prof David Phillips CBE *(Royal Society of Chemistry)*
Dr Fabio Pulizzi *(Nature Materials)*
Dr Subramanian Sankaranarayanan *(Argonne National Laboratory)*
Dr John Stevens *(Baker Hughes)*
Ms Marianne Talbot *(University of Oxford)*
Mr Piero Vitelli *(Island 41)*

Contact Details

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Industry Partner Contact

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Dear Mariellanne...

Mariellanne answers all your dilemmas (within reason)

Real life Mariellanne (not in disguise)

Dear Mariellanne: I am an engineer–to–be looking for a PhD, so I am not sure whether the TSM CDT programme is best for me: it involves gaining an additional master's, and seems very physics–oriented. Would I have any chance of doing anything useful here?

The CDT's motto is '*bridge the gap*'. There is a huge barrier between Physics and Engineering that is difficult to breach, and that is why the CDT recruits both engineers and physicists. Bridging the gap is not an easy thing—engineers might know nothing about quantum mechanics, whereas physicists will ignore everything about solid mechanics. Thus, the first year MSc is mostly about offering both enough training to be able to understand one another. Afterwards, one can conduct research in fields as apart as statistical mechanics or real life applications in fluid mechanics, and yet, thanks to that MSc, be able to grasp each other's work: how many engineers can do that?

Dear Mariellanne: The fact that the TSM CDT is based in London is definitely a plus, but it does seem quite a lot of work... Is joining it a good way to enjoy the thrilling metropolis of London?

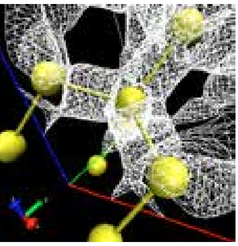
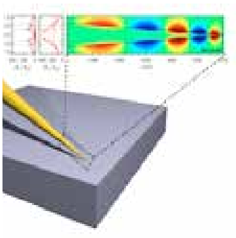
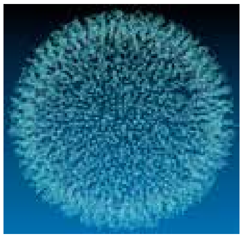
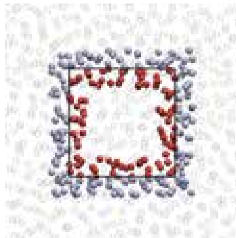
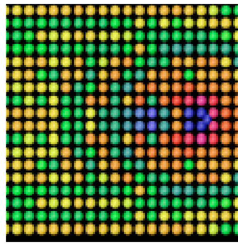
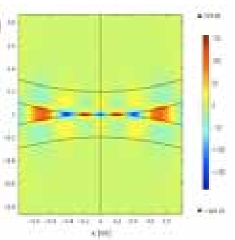
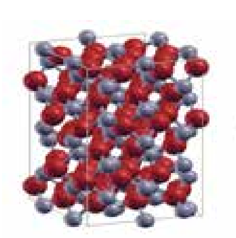
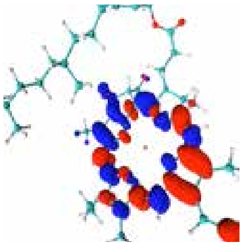
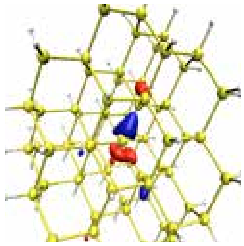
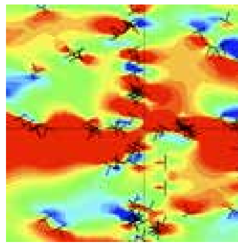
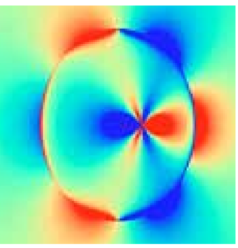
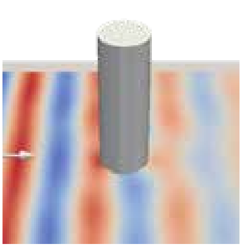
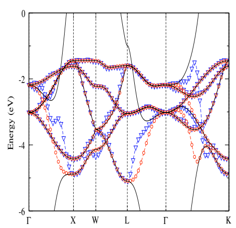
The serious answer to this question would go along these lines: '*One does not join a PhD to party...*' Of course, if that's the only thing you are looking for, I would advise going to Caribbean instead where, on top of everything, the weather is milder (except in hurricane season). Which said, living in a cultural hotspot such as London does have its advantages, and it's not all about work all the year around—we definitely get as much free time as people working in the City, so chances are you will get to enjoy London while working for your PhD.

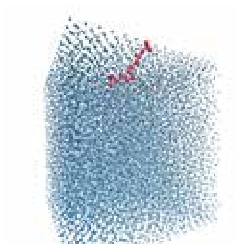
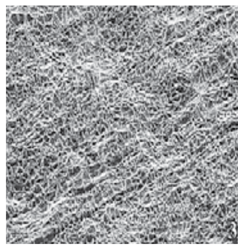
Dear Mariellanne: I am interested in theoretical physics, so dealing with engineers or materials scientists scares the hell out of me. Would the TSM environment force me to abandon the epicycle of Mercury for more mundane endeavours?

One of the best things about TSM is the freedom it offers to choose or design your own PhD—except for experimental projects, you can essentially work on anything you want with any of the 6 academic departments that take part in it. Current students work in fields ranging from, indeed, engineering and materials science, to highly theoretical projects in condensed matter physics or statistical mechanics. Thus, fear not! TSM is as good an option for those seeking pure theory as string theory itself.

Imperial College
London

Theory
Simulation
Inspiration

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