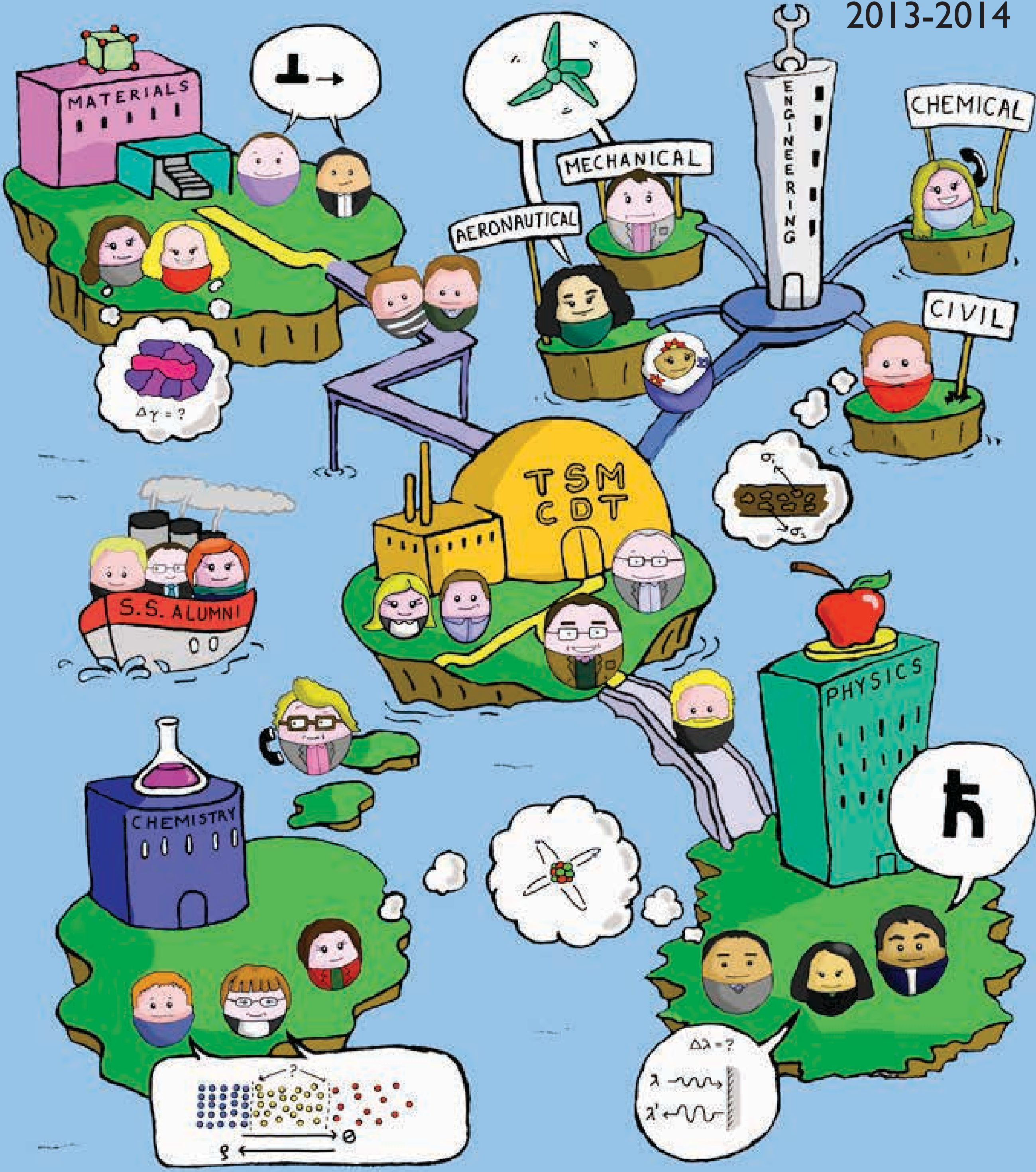
Annual Report

2013-2014



Centre for Doctoral Training in Theory and Simulation of Materials

"It's not that scientists are more honest people, it's just that nature is a harsh taskmaster."

—Noam Chomsky, A Life in Dissent, 1992.

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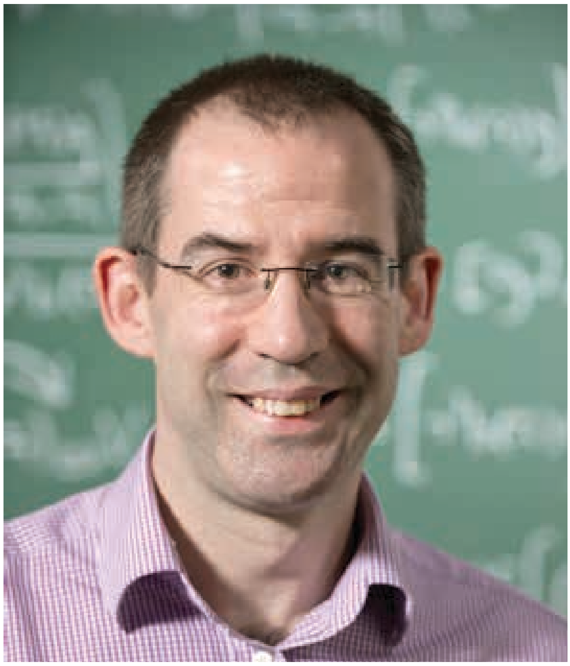
London, November 2014

Director's Foreword

OVER THE past few years I have occasionally observed some similarities between a Centre for Doctoral Training (CDT) and a family – perhaps the most obvious is that relationships lie at the heart of both. But each cohort of students also has its own unique collective personality: like the eldest child, our first cohort benefited from tremendous attention and suffered from the mistakes of our inexperience. Our second seems much more relaxed and (rightly) self-confident. And as a family progresses through phases in its life, so does a CDT. Over the last academic year our CDT has celebrated the passing of two major milestones in its corporate life.



The first of these was watching our first cohort of students submit their dissertations (all on time), passing their vivas and moving on to the next stage of their careers. These include jobs with well-known companies such as Rolls-Royce and IBM, post-doctoral research positions, the Civil Service and starting up a company. Cohort 2 (the ever-competitive younger sibling) is already hot on their heels, with two students winning independent research fellowships and two moving to post-doctoral positions at Cambridge and MIT. We take great pride in their successes and delight in seeing each one flourish as an individual.

However, our home in the Whiteley Suite feels anything but an empty nest; this autumn we welcomed our sixth cohort of students – one of our largest yet. The start of a new academic year is always a significant moment but 2014–15 is especially poignant because our new arrivals are the outcome of the decision by the Engineering and Physical Sciences Research Council (EPSRC) to award our CDT funding towards a further five cohorts. The support of Imperial and our growing network of external partners was vital to our success, providing additional funding for studentships that will give us more flexibility to recruit and train outstanding students who wish to apply their theoretical talent and mathematical flair to tackle challenges in materials science that will have a lasting impact on our society and economy.

The coming year will see some changes to the delivery of our training as we implement the proposals from our funding application. However, the mission and ethos of the EPSRC Centre for Doctoral Training in Theory and Simulation of Materials will remain the same. As in previous editions, this third annual report has been written and edited by the students themselves. I hope you enjoy reading their own account of their achievements.

Prof. Peter Haynes

Contents

Masters of Materials

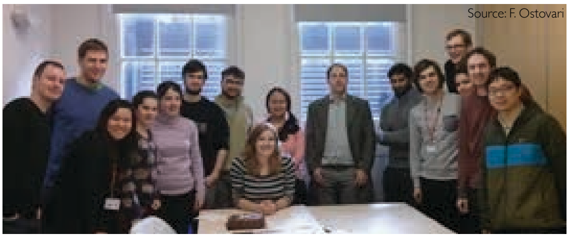
***MITESH PATEL** on Cohort 5 living in a material world. A report of Cohort 5's first year.*

Source: Flickr--University of Exeter

THE TSM MSC experience is a unique challenge: an intense year with a myriad of opportunities to develop and refine a spectrum of skills. Personally, it is very interesting to see, for example, how a physicist approaches an engineering problem or vice versa. Nowadays, materials research is somewhat synonymous with trendy terms such as 'interdisciplinary' and 'multiscale'. But this notion becomes much more meaningful during the TSM MSc when you actually have to engage with problems in physics, chemistry, materials science and engineering. In doing so, you begin to appreciate the culture in different departments as well as the richness of this diversity.

As the acronym TSM implies, the MSc is designed to expand your theoretical and computational materials repertoire with everything from density functional theory to finite element simulations. Not only do you become more versed with your mathematical and programming abilities but you also become more organised and efficient because of the sheer volume of content you have to absorb. On top of this, you learn from scientists and engineers who are at the forefronts of their field of research and are eager to train the next generation: you!

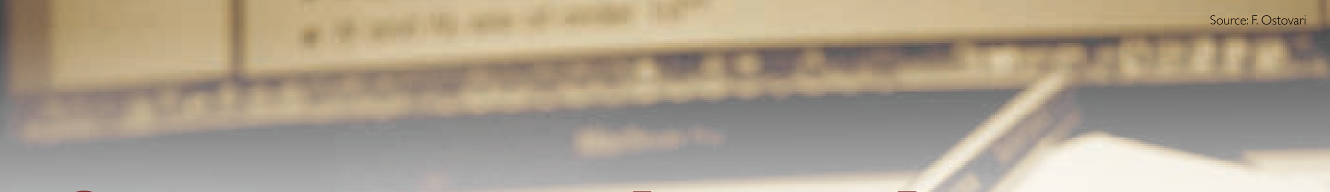
Fortunately, the journey is more than just a route to a degree. You are in a cohort of very able students from various academic and cultural backgrounds. The cohort is supported by a mentor; their role is to ensure that your experience is nothing short of exceptional. Throughout the year, you work together, you eat together and you grow together. You form good friendships and learn from one another in your development towards being a well-round scientist and human being. For us, a consensus highlight of the year was the trip to the US to attend our first international conference; I am sure that all members of our cohort fondly reminisce about the amazing time that we shared in San Francisco.



Source: F. Ostovari

Cohort 5 enjoys lunch with their mentor, Daniel Balint.

The TSM-CDT model provides a stimulating academic and social culture, and it does both exceptionally well. During the TSM MSc, the focus is very much on you as you refine many valuable skills relevant for a career in either research or industry. The hope is that you become the jack-of-all-trades (-modelling-materials) and the master of some. Moreover, being a part of the TSM-CDT, you will see that it is a wonder of opulent science, persevering minds and the vibrant network that binds them.



Source: F. Ostovari

Scientists in the Making

We asked our current crop of students what it means to do a PhD in the CDT.

Q) *What project are you working on?*

Multi-scale modelling of intermolecular charge transport in dye-sensitized solar cells.
Valérie Vaissier (Cohort 2)

A molecular mechanism of viscoelasticity in aligned polyethylene.
Ali Hammad (Cohort 3)

Ab initio modelling of ferroelectric thin films, which usually find application in nano-electronic devices.
Andrea Greco (Cohort 4)

Q) *What are the main highlights of your CDT experience?*

The very good courses during the MSc year which widened my experience in the theory and simulation of materials.
Jawad Alsaei (Cohort 2)

The privilege of working with some truly brilliant people.
Benjamin Kaube (Cohort 3)

I really enjoyed the Master's year of the CDT, I think the structure was really good and it really motivated people to work together.
Andrea Greco (Cohort 4)

Q) *What are the main challenges when working in an interdisciplinary environment?*

The CDT motto is 'spanning length and time scales' and this brings unique challenges. For me, it meant I had to do a lot of coding in order to create something that will do what I wanted.
Joshua Tsang (Cohort 2)

Making links between different areas that have traditionally been treated as separate is a significant challenge. Having said that however, persevering with such interdisciplinary projects is very rewarding.
Ali Hammad (Cohort 3)

The main challenges for me were to try and understand to what extent physical information can be transferred from one length scale to the other.
Andrea Greco (Cohort 4)

CDT students discussing their research

Source: M. Khawaja

Q) *How do you feel the CDT PhD compares to other programmes?*

The CDT invested in me as a person rather than just as a scientist. It also provided me with a stable framework within which to grow and achieve my goals. I feel this greatly enriches the PhD experience.
Valérie Vaissier (Cohort 2)

I think it is much better because the specialised MSc allows for a more natural transition into the PhD, especially if you go on to work in a different field from that of your undergraduate degree. You also get to know a much wider range of students and staff.
Stephen Burrows (Cohort 4)

Q) *How well has the CDT experience prepared you for your future career?*

Very well, the "extra-curricular" events were, on the whole, extremely beneficial.
David Trevelyan (Cohort 2)

I feel that the technical training, complementary transferable skills and the professional network fostered by the TSM CDT have left me well prepared for my career ahead.
Benjamin Kaube (Cohort 3)

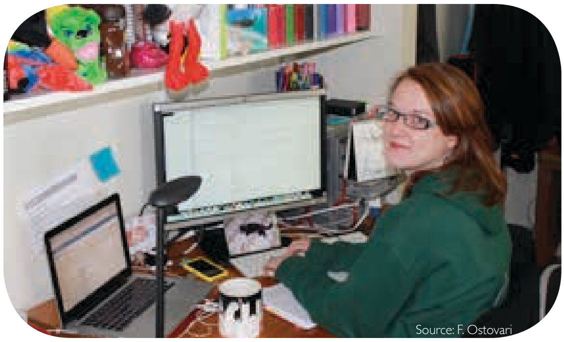
I think overall the training has been very good. I am not sure what my future career will be yet, but I feel that at the end of my PhD I will be in a good position to make the right choice for my future.
Andrea Greco (Cohort 4)

Q) *If you could summarise your CDT experience in two sentences, what would you say?*

Two words are enough: absolutely brilliant!
Valérie Vaissier (Cohort 2)

My experience of the TSM CDT has been overwhelmingly positive. I have relished the challenges and opportunities that the CDT has afforded me!
Benjamin Kaube (Cohort 3)

I think it is great that CDT students really feel like part of a "family", where everyone shares, communicates and develops their love for theory and simulation of materials.
Andrea Greco (Cohort 4)


Source: F. Ostovari

Valérie Vaissier (Cohort 2) hard at work

Q) *If you were to describe yourself as a material, what material would you be?*

Oobleck. Because I can shape myself to many situations but become stone if you push me to do something I don't approve of!
Valérie Vaissier (Cohort 2)

Aerogel, I gel well with other people and have been known to be full of hot air!
Benjamin Kaube (Cohort 3)

I would say carbon fibre, very light but also very resistant.
Andrea Greco (Cohort 4)

Source: forums.deeperblue.com--marginatus

Viscoelasticity in Aligned Polyethylene

Research Highlight

Ali Hammad elucidates the mechanism behind super-strength polymers, which may prove useful in areas as diverse as defence and medicine.

Aligned polyethylene is a lightweight but incredibly strong material, with a Young's Modulus comparable to steel. This makes it ideal for a broad range of industrial applications, including ropes for offshore drilling and the maritime industry. However, the actual strength of the material is below its maximum theoretical strength, and plastic behaviour is also observed. In this research project, we begin to understand how plasticity arises in the material, and how the mechanical properties of the material can be improved.

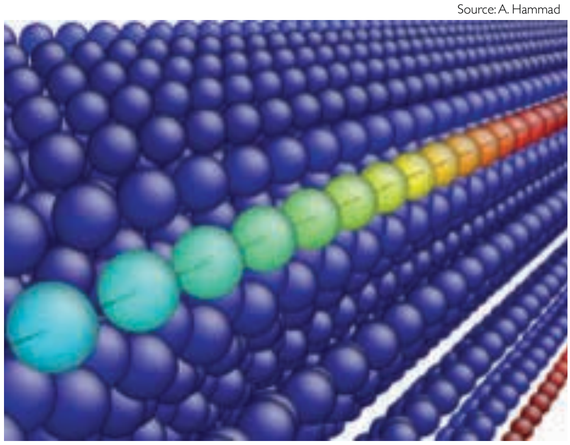
We explain the mechanical properties of aligned polyethylene through the formation, interaction and movement of solitons, which are localisations of strain in molecular chains, associated with a double vacancy of two adjacent CH_2 groups. These mechanisms arise from the semi-crystalline microstructure of the material, as the solitons nucleate from interfaces between the crystalline and amorphous regions of the material.

When the material is heated to room temperature the solitons disassociate into 'twistons' which are single vacancy defects accompanied by a 180° twist in the polyethylene backbone. These defects can annihilate with the interfaces between crystalline and amorphous regions, potentially explaining how the material retains a memory of its original length after deformation.

The theoretical framework that we propose may be transferable to other aligned polymers such as poly(*para*-phenyleneterephthalamide), better known as 'kevlar'. Further continuation of this work may result in the design of aligned polymers with higher elastic limits and smaller hysteresis.

We intend to publish this work as three papers in series. The research effort was a collaboration involving many people: Prof. Lorenzo Iannucci and Stefano Del Rosso (Dept. Aeronautics), TSM-CDT students Thomas Swinburne (Cohort 2), Hikmatyar Hasan (Cohort 6) and Mohammed Khawaja (Cohort 3), and my principal supervisor Prof. Adrian Sutton.

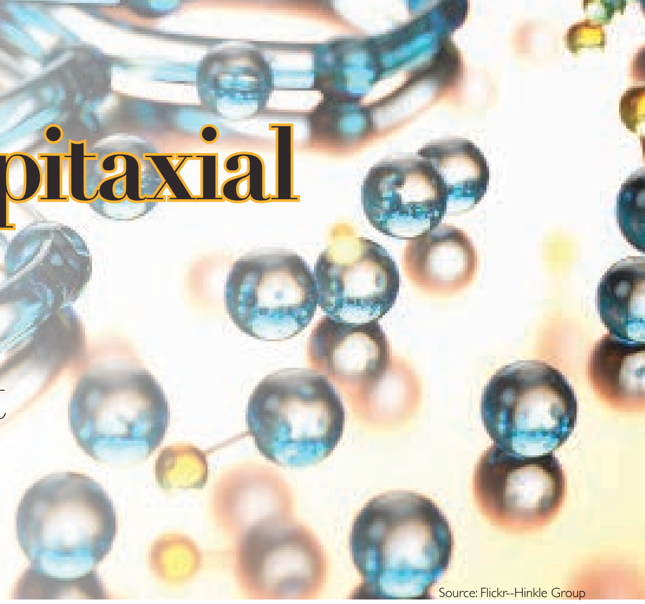
Source: A. Hammad



Soliton in a molecular chain of polyethylene

Simulating Epitaxial Graphene

Research Highlight

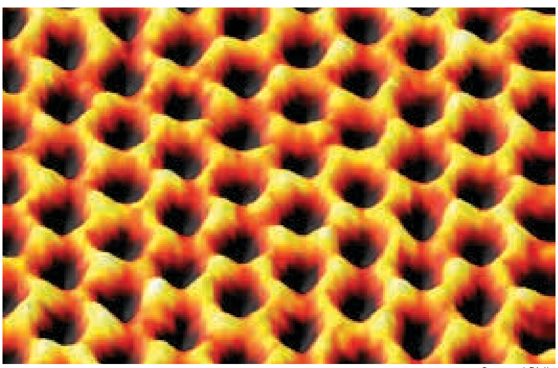


Source: Flickr--Hinkle Group

***Joel Posthuma de Boer** takes a look at the science of growing graphene.*

SINCE THE FABRICATION OF GRAPHENE in late 2006 by Andre Geim and his team at the University of Manchester using the so-called "scotch tape" method, interest in epitaxial growth processes has been rekindled by many groups who see it as a promising technique for the production of industrial quantities of graphene. This work includes experimental advances in graphene fabrication by epitaxial growth as well as a number by theoretical groups striving to understand the atomistic mechanisms that govern graphene formation.

The main tools at the theorist's fingertips range from quantum-mechanical calculations to obtain lowest energy structures to methods which are able to predict dynamical behaviour at differing levels of accuracy. Fully spatially resolved methods such as Kinetic Monte Carlo simulations (KMC) are often too computationally expensive to be employed in the low flux and high temperature conditions in which the growth of graphene usually occurs. Instead we use spatially independent models such as rate equations which, although simple, can successfully capture important physics that are of some use in understanding growth mechanisms.



Micrograph of graphene

Source: LBNL

The input parameters can be taken directly from *ab initio* calculations or obtained by fitting the solutions of the rate equations to experimental data. We researched the latter situation, introducing a novel method for the exact calculation of gradients that can be used to obtain the best agreement between the numerical solutions of rate equations and experimental data. This analysis therefore provides a more complete description of early stage graphene growth on iridium.

Joel is supervised by Prof. Dimitri Vvedensky (Physics), Prof. Ian Ford (UCL Physics) and Prof. Lev Kantorovitch (KCL Physics).

Confined Ionic Liquids for Electroactuators

Research Highlight

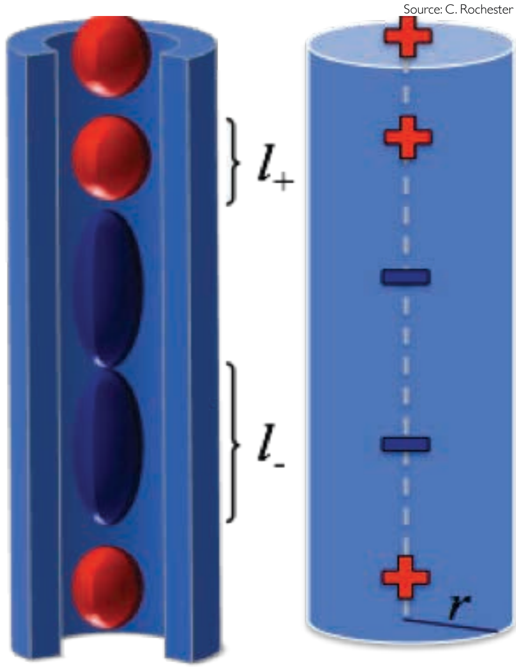
CHRIS ROCHESTER investigates energy storage at the nanoscale, the subject of his most recent paper "Interionic interactions in conducting nano-confinement"*.

THE AIM OF MY RESEARCH is to develop an understanding of energy storage in confined nano-structures. I focus on explaining devices called 'supercapacitors'. These supercapacitors consist of two electrodes wetted by an electrolyte. Energy is stored via the formation of a double layer of counter ions, from the electrolyte, on the electrode surface. This process is reversible, giving supercapacitors a long lifetime, and has the capability to store much more energy than a regular capacitor.

The energy stored is proportional to the size of the double layer and thus the surface area of the electrode. One way to increase the surface area of the electrode, for a given volume, is to increase its porosity. However, as the electrode becomes more porous, ion confinement on the nano scale - within the electrode - starts to introduce new effects visible at the macro scale.

I have one paper published on the topic describing how ions are electrostatically screened in extreme confinement. This work has been recently supported by independent

Source: C. Rochester

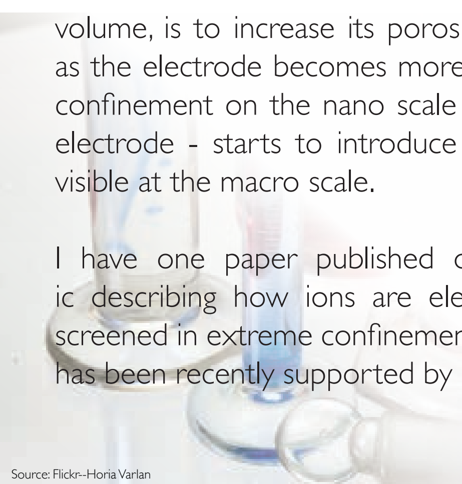


Ions confined in a nanopore

Density Functional Theory (DFT) calculations conducted in Germany. I am also currently in the process of writing two other papers: one, a model of electrode swelling that provides a mathematical description of previously unexplained experimental observations; the other, suggesting how to optimise electrodes to increase total energy storage.

Chris is supervised by Prof. Alexei Kornyshev (Chemistry) and Dr Gunnar Pruessner (Mathematics).

** Rochester, C.C.; Lee, A.A.; Pruessner, G.; and Kornyshev, A. A., Chem. Phys.Chem, 14(18), 4121-4125(2013)*



Source: Flickr--Horia Varlan

Source: Flickr--coloneljohnbritt

The Rheology of Complex Fluids

Research Highlight

***Stephen Burrows**, of Cohort IV, goes with the flow and discusses his work on complex fluids.*

CONSIDERING IT TOOK me an hour to write the first sentence for this article, it's no surprise that deciding on a research direction for my PhD took a long time. Ultimately, I decided not to venture into the world of electronic structure, but to look for a PhD project with a fluid dynamics focus.

The primary computational tool used in my project is the lattice Boltzmann method, an increasingly active area of research. Instead of dealing directly with quantities like velocity and pressure, these are extracted from a particle velocity distribution function which is constrained to a lattice. Even though it uses an adapted form of the Boltzmann equation, the method can be viewed as a solution algorithm for the Navier-Stokes equations of fluid dynamics. It is well suited for massively parallel computing, meaning computational resources can be used efficiently. The method can be adapted for multiphase flows using a free energy approach, for which we can use molecular dynamics simulations to obtain parameters such as surface tensions and solubilities.

As for the application, the initial plan was to simulate the flow of fluids through porous media. However, this area is already being comprehensively studied at Imperial, so I felt a change of direction would be beneficial. This removed the chance of collaboration with the original industrial partner, but allowed us the opportunity to accept some funding from an EU FP7 project related to interfaces in a new type of flow battery.

Designers of these batteries wish to pump a suspension of $LiCoO_2$ particles through narrow, winding channels allowing the exchange of lithium ions between reservoirs. The aim of my current work is to determine how and why the particle size and shape affects the energy required to pump the fluid around the system. This is an interesting problem because once you reach a certain amount of particles in the fluid, the fluidity or 'flowability' plummets quickly, making the suspension impossible to use. Most analytical theories are only valid at low volume fractions.

Source: S. Burrows

So far I have been working on simple problems involving circular or spherical particles with quite predictable behaviour. I will be presenting some initial results at a workshop in Ulm, Germany in November. However the real core of the project lies ahead, as the next stage involves simulating non-spherical particles under a range of shear rates.

Stephen is supervised by Dr Edo Boek (Chem. Eng.) and Dr Fernando Bresme (Chemistry).

From Science To Society

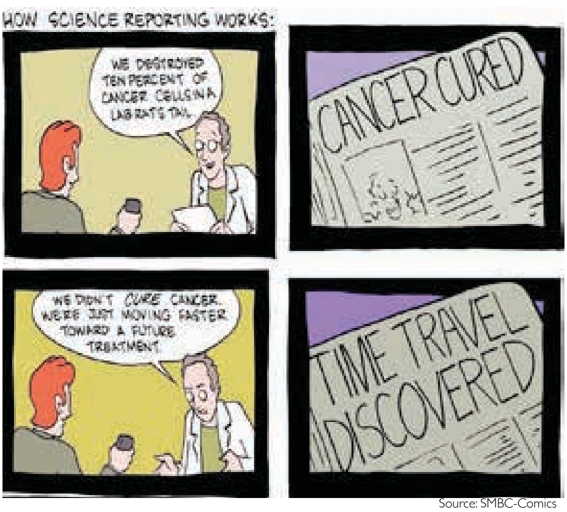
Masterclass

Students of the TSM-CDT were paid a visit by* Dr Matthew Brown *of the Royal Society of Chemistry.* Ali Hammad *reports.


Source: Dr M. Brown

EARLIER IN FEBRUARY this year, we had the pleasure of receiving a Masterclass on Science Policy and Communication with Dr Matthew Brown (pictured), who currently works as the Head of Communications and Campaigns at the Royal Society of Chemistry. Since completing his PhD in computational materials science at the University of Cambridge, Matthew has gathered a wide-range of experience working in two government departments (DECC, DEFRA) as well as the Confederation of British Industries (CBI).

The link between his background in the simulation of materials and his employment in Science Policy and Communication was especially relevant to the students in the TSM-CDT. Being engaged in a PhD programme, we all had questions. What skills can you transfer from a PhD to the interactive world of people and employment? What must you unlearn from a PhD to become effective at the Communication of Science to the public, or to work with people from various backgrounds?



Source: SMBC-Comics

The Masterclass was delivered in an informal way, with students engaging with Matthew during his talk. We all learnt that the intellectual rigour of a PhD is transferable to many walks of life. It is essential that one understands something properly before delivering it. Matthew recounted from his own experiences that this practice helped him solve many problems during his working life. However, he also informed of us of the need to avoid being "too correct," that sometimes good is good enough. He stated that he had to unlearn this style of thinking that came from his PhD.

After the Masterclass there were so many questions that we had to continue the discussion in a local pub, where the students continued to grill Matthew. Overall the Masterclass was an excellent learning experience from which we all benefited.

Showcasing Success

Internal TSM-CDT Conferences

***Andrew McMahon** reports on the CDT's very own world-class conferences.*

On 24th June 2014, all of the TSM-CDT cohorts, as well as members of staff and members of our International Advisory Board (including the keynote speaker, Professor W. Craig Carter from MIT) were brought together in the Royal School of Mines for the first TSM Annual Conference. The premise seemed simple enough – get everyone involved in the CDT into a room and share what we've been up to over the past 5 years – the results however, proved spectacular.

The day was an excellent showcase of the abounding success of the CDT and included world-class scientific talks given by members of Cohort 2, a thought-provoking poster session showcasing the work of Cohorts 3 and 4 and many interesting discussions over coffee breaks and lunch. To cap it off there was then the awarding of a series of well-deserved prizes!

Professor W. Craig Carter was keynote speaker at the TSM-CDT Annual Conference.

The members of the CDT Advisory Board who were present, as well as our own Director, Assistant Director and Chairman (Peter Haynes, Arash Mostofi and Adrian Sutton) were all extremely impressed and praised the fantastic quality of the work that was on show.

To conclude the day, we were all treated to an excellent talk from Professor Carter on his latest research on the mechanical degradation of materials used in battery technology. Professor Carter's research is a perfect example of how theoretical materials science can be used to benefit society, one of the founding tenets of the CDT.

Cohort 5 also presented their work as the final part of their Masters projects in the annual MSc conference in September. After an impressive array of talks we had the pleasure of attending a TYC seminar by our guest of honour Dr Gabor Csanyi from the University of Cambridge.

Beñat Gurrutxaga-Lerma (Cohort 2) presents his research at the TSM-CDT Annual Conference.

Dr Csanyi discussed advanced probabilistic inference techniques applied to multi-scale materials simulation. It was a tour-de-force of mathematics and theoretical physics that left us all eager to learn more. The talk also highlighted to all present the importance of our CDT in training a new generation of scientists in the theory and simulation of advanced, technologically relevant materials.

Catalysing Interest

Source: JM

Drew Pearce *reports on the time Cohort 5 downed tools to head out to see research within industry with a visit to Johnson Matthey.*

Donning lab coats, goggles and safety shoes, Cohort 5 went to visit Johnson Matthey (JM) in order to get a flavour of modelling in the wild. JM is a multinational company with a strong research focus and one of the main producers of catalytic converters. During the visit we toured the catalytic converter assembly line. This involves coating a frame with a wash-coat, designed to convert harmful toxins into more inert compounds. We then proceeded to brainstorm possible ways of modelling the coating process. As in many real world problems there were many possible approaches each with their own pitfalls. Such an understanding could be used to increase cost-effectiveness and reduce waste.

The physics instincts kicked in and we quickly simplified it down to spherical particles in a single solute. A lively debate followed about the merits of a model so simplified. Eventually, it was decided that it could provide a qualitative understanding before building in extra complexity. It was inspiring to see the methods we learn about being used to tackle real practical problems. We were also interested to see how research worked outside the academic context and learned about practical situations where materials modelling is able to cut waste leading to a more sustainable product and ultimately a cleaner, healthier planet.

Source: JM

So, in conclusion, we were able to see that industry can offer exciting scientific and intellectual challenges, all in the context of creating a more sustainable, greener planet Earth. We were also able to see how our skills can help solve a real world problem and how we can integrate ourselves into industrial research teams and beyond.

Industrial Relations

The CDT enjoys a very close relationship with our industrial partners. Here is what some of our industry funded students think.

Source: F. Ostovari

Source: F. Ostovari

What are the challenges and benefits of working with industry?

The challenges are those one might expect: the right to publish, the goals of the project must match the goals set out by the industrial partner, and working with a collaborator outside of academia. The benefits are having all those things an industrial partner can offer that a university cannot: a unique perspective on the work of the company via industrial contacts, the chance to get work experience via a visit or placement with the company, and of course a wide range of career opportunities for the future.

***Adam Ready (Cohort 4)** is working in collaboration with Rolls Royce for his PhD on cold dwell fatigue in Titanium.*

How useful is it having an industrial connection during your PhD?

It's great having someone well-versed on the practical side of things to discuss ideas with. For example, it turns out that a simple solution to my particular problem (elastomer seal failure in oil drilling) is to slow down the drilling process, spending an extra day or so while wrapping up the operation to ensure that the seals don't fail. But it turns out the cost associated with doing so would be astronomical — hundreds of thousands of dollars per day — and therefore it's not exactly fiscally feasible. Having an industrial project forces you to confront realities that a more theoretically minded physicist might consider merely mundane or inconvenient.

***Musab Khawaja (Cohort 3)** is working in collaboration with Baker Hughes for his PhD on elastomer seals for use in oil drilling.*

Source: Flickr--EnergyTomorrow

Source: Flickr-- Daniel Pietzsch

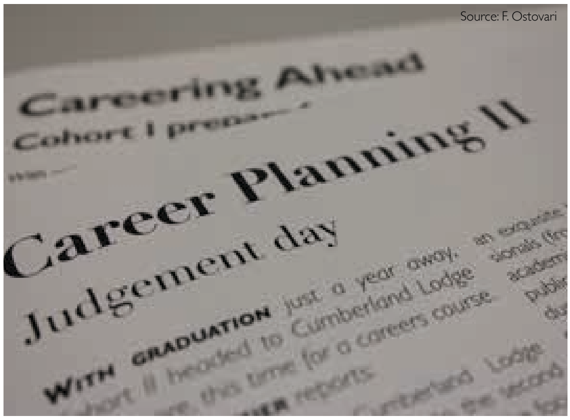
The Best Laid Plans ...

Career Planning

***Vincent Chen** gives us his view on the residential career planning course, and how it made him think about his future after the CDT.*

SET IN SERENE, picturesque gardens next to the University of Warwick campus, the Arden Conference centre served as the venue for the 2014 edition of the Careers Planning Course. The three-day course kicked off with an introduction by course organiser Prof. Adrian Sutton, who first placed academic careers into perspective, and opened our eyes to the wide range of other options — it turns out that you can use scientific thinking in all walks of life. Following this important message, there was time for some lively participation from the students, which continued throughout the whole course. There were a handful of small group discussions interspersed among talks given by the enthusiastic and knowledgeable tutors.

Of course it was important to get our CVs and interview techniques right, and much of the course was dedicated to that. The most interesting part of the course however was during the second day, where six guests from a variety of employment sectors kindly joined us to present their life stories and provide us with some insight into the opportunities available to us. In addition, we



Source: F. Ostovari

were able to meet each guest individually in our small groups, which gave us more of a window into their experiences. To finish off the course, each of us participated in mock interviews, both as interviewer and interviewee.

The Careers Planning course certainly exposed us to the wide range of available career opportunities, both within and outside of academia. It was also a gentle reminder for all of us to begin serious planning for the next big step.

Authentity, Ethics and Science Communication

Or 'how I learned to stop worrying and love professional skills'.

Source: Flickr--Rusty Sheriff

As part of their training, TSM-CDT students attend certain courses to provide skills that will help them stand out from the crowd as they continue their career.

Science Communication

Straight after the New Year, members from Cohorts 2 and 3, along with other UK postgraduate materials students participated in the three-day workshop in science communication at Cumberland Lodge. The aim of the course was to teach scientists how to effectively engage the public with their research and to provide first hand insight into various aspects of media; the highlight would be the recording of a radio feature at the end of the course.

Three enthusiastic organizers made this possible: Dr. Claire Ainsworth presented the foundations of science journalism and Gareth Mitchell (from BBC Click) and Robert Sternberg were the radio and TV specialists, respectively. After introducing what makes high quality news features in TV and radio, they allowed the students to get hands-on in recording their own short features. This was followed by editing sessions where the raw recordings were pieced together. Having had a brief grounding on the basics of science communication from Gareth, the excited attendees travelled to BBC Broadcasting House (London) on the final day to record their twenty-minute radio shows.

Authentity

The Authentity course was one of the more unusual workshops. Working on a group project under time pressure, all the while learning about what makes a group effective was exhilarating. The terms growth and personal development are too often bandied about when discussing Professional Skills courses but this course really did develop us as individuals. It caused us to reflect on ourselves and how our behaviour affects others. Rather than focus on a particular skill (e.g. 'Team Work') it focused on giving participants the ability to reflect and develop the skills they wanted to themselves.

Ethics

The questions most scientists and engineers consider are: Can we do it? and Can we understand it? Very rarely do we consider the ethical dimension. The questions Should We? and Is this ethical scientific practise? are considered through a series of ethics courses delivered by Ms Marianne Talbot of Oxford University 's Department of Continuing Education. The grey areas of ethics are explored and discussed in an open, inclusive environment. These discussions help us become more mindful of the choices we make and how it will affect wider society. A truly vital skill that is perhaps often overlooked.

Source: The Open University

Pint of Science

Source: Flickr–Simon Cocks

***Max Boleininger** shares his experience of the student-run initiative to get scientists and interested members of the public talking over a pint.*

A DARK AND MURKY PUB in the heart of London. For possibly the narrowest entrance in all of the city, the inside is surprisingly spacious. The smell of fish and chips, cottage pies, and ale lies heavy in the air. The crowd barely fits into the room, crammed around undersized tables.

In short, nothing out of the ordinary. Were it not for the curious people gathering around a banana-powered speaker cone, blasting "Smoke on the Water" to bring corn-starch into resonance. Or dry-ice powered bubbles, filled with clouds, gently drifting through the room. And what about the four Imperial scientists pitching their favourite material to the patrons, from composite material cake, to non-Newtonian ballet shoes?

Pint of Science is an annual student-run festival that aims to make science accessible and fun for the public by bringing scientific research to the cosy atmosphere of a pub over three evenings. Our goal is to bridge the gap between the public's perception of academic research, and the very different reality we know. For this reason we bring the science out of the university, and put it into an open environment where people can let their natural curiosity take over.

We invited six researchers from Imperial College to hold talks on themes such as solar influences on climate, glass in biomedicine, and materials engineering. This year we also brought Simon Foster's brilliant science demonstrations to our pub, which were mostly run by TSM-CDT students. The evenings were wrapped up with a science-themed pub quiz, with trivia questions that would make even a senior researcher scratch his head! The reception was fantastic — the talks sparked dialogue between audience and scientist that would last well over half an hour. With the majority of our guests coming from a non-scientific background, we managed to present our field in a more accessible light, thanks to funding from the TSM-CDT that made the event possible!

Source: M. Boleininger

Source: Flickr-- Peter Jepsen

Magnetic Moments

***Marc Coury** tells us about his obsession with superconducting magnets and how this has helped his scientific outreach.*

Ever since I first saw one of those black circular pieces of ceramic floating in mid-air I have been fascinated by superconductors. The first time I saw it, at the tender age of 17 at the University of Bath, demonstrated by Dr Peter Ford MBE, I was shocked, amazed and intrigued all at the same time. The world really holds surprises and it is through searching for understanding that you can discover magic like this. The surprise and awe I felt the first time comes back every time I get to show a superconductor floating in mid-air to a visitor to Imperial College London.

The MBE after Dr Peter Ford's name was awarded to him for his services to science and higher education through outreach. Outreach really is an important part of science. It is a way to give back to the public, which supports a large proportion of our research and teaching, and to show them what we are doing in universities. It's also a good way to get young people interested in the sciences, to realise their importance and to consider studying them at university.

Not only that but it's also really good training as it gives scientists an opportunity to improve their ability to communicate science. Simon Foster, the TSM-CDT and Physics Outreach Officer does a really good job of making a ton of opportunities available to get involved in outreach and a lot of students in the CDT choose to do so.

Being a part of the TSM-CDT I've received a lot of support for doing outreach. I've organised stands at the Imperial Festival 2013 and 2014, the Research in Motion week 2013, the Fluid Thinking Imperial Fringe event in 2013 and participated in outreach during many open days.

As I find superconductors so fascinating I have done a lot of outreach based on them. For the Imperial Festival 2013, with the help of Leon Vanstone, Famelab UK winner 2013, I built a track of 3,000 magnets on which to float a superconductor (pictured). That was cool and fun, but the magnetic field of the track wasn't strong enough to float the superconductors very high. So, I spent money from the 2013 TSM-CDT Outreach Prize on another 6,000 magnets and, with the help of Ali Hammad and Jassel Majevadia, upgraded the magnetic track to 9000 magnets in time for the Imperial Festival 2014.

Marc's superconducting magnetic track uses 9,000 magnets!

Source: M. Coury

This impressive track is available for use for outreach demonstrations at Imperial College London and you can see a video of it here:

https://www.youtube.com/watch?v=HTXfSfnMRpQ

Hermes

Drew Pearce *reports on Hermes 2014 and the plans for its inevitable extension into 2016 and beyond.*

It's been two years since students from the TSM-CDT and the Thomas Young Centre (TYC) ran the first student-developed international summer school., Hermes 2012. It was a rousing success and inspired a coalition of attendees, including other TSM-CDT and TYC students, to organize another: Hermes 2014. The unique element to Hermes is that it provides two sets of people with very special opportunities. First, attendees are taught about theoretical and computational techniques from the 'heavyweights' of the field. It also provides key personal development in areas often lacking in a PhD program, such as communication skills. They do all this within an international framework: over 40% of attendees originated from outside of the UK, from a wide array of continents.

Source: M. Coury

Mark Miodownik speaking at Hermes 2014

Throughout Hermes, attendees were put into groups to discuss the masterclasses and to help develop their individual task for the summer school. In 2012, this was an educational science video and in 2014 it was a presentation without slides or notes, on one of the topics of the masterclasses to a panel of peers and judges. The standard was very high and all the judges were impressed, including materials media magnate Mark Miodownik.

Attendees of Hermes 2014

Source: M. Coury

The second key group is the organisers. Organising a summer school is no easy task: it involves managing a team of people, securing funding, dissecting the literature to find the current hot topics and finding suitable world-leading academics to lead the masterclasses. All of these are opportunities for the individuals to develop skills that they otherwise would not have. It provides significant scope for personal development and gaining skills that will serve them well, regardless of the path they end up choosing.

Source: M. Coury


Source: M. Coury

Indeed, the Chair of Hermes 2014, Marc Coury, said *"Through leading a team I have learned a lot of really important interpersonal skills, such as realising that leadership is actually a form of servitude, i.e. facilitating. I've also learned how to effectively delegate tasks. That may sound banal, but in fact there are some subtleties: people will complete a task to much higher standard if they feel that they own that task; also tasks have to be matched to the interests and skill sets of the people and in some cases be chosen so as to help them to improve their skills. It has forced me to consider my own strengths and weaknesses in a team and how to improve upon them. Finally, I've learnt to trust people to do things well."*

I was an attendee of Hermes 2014: It has educated me about techniques of simulating materials beyond the narrow scope of my PhD, it has improved my communication skills and, most importantly, my confidence to use them. Finally, it has inspired me to pass those opportunities forward. As such, alongside a whole new team of eager organisers, I will be leading Hermes as we attempt to become a permanent biennial fixture on everyone's calendar, starting with the next event in 2016. We aim to continue the trends of developing attendees' skills in both 'hard science' and 'core skills' that will help them produce high quality research, communicate their research, work effectively with others and grow as individuals.

Hermes 2016 Summer School

This is no mean feat and I have absolute confidence that our new team can build upon the foundations of previous years and deliver a truly world-class summer school. Utilising the support and input of leading academics, key players in industry and of course the TSM-CDT. We are currently busy developing an innovative way to test, stretch and build the attendees' communication skills. This could involve utilising new ways of representing data to make a case or convince a panel of judges that their idea is worthwhile and feasible. Whatever we decide, I'm sure it will be fun and educational and alongside the other activities will make Hermes 2016 as good as the previous two, inspiring a new generation to develop Hermes 2018 and beyond.


Source: M. Coury

Googleplex

***Fabian Renn-Giles and Niccolò Corsini** tell us about their entrepreneurial exploits.*

In April 2014, we took part in the Catalyst Grant competition — hosted by the TSM-CDT — and pitched our start-up idea to a panel composed of executives from Digital Science. Catalyst Grants provide vital funding and resources to turn innovative scientific software ideas into working prototypes. We presented CrowdSense (www.crowd-sense.org), our software project for collecting distributed sensor data for the sciences. It was a challenging and hugely rewarding experience not only for the learning process of turning an idea into a reality but also for the valuable feedback and encounters along the way.

As a result we were very fortunate to be invited to the GooglePlex in California in August, courtesy of Digital Science, for a one-of-a-kind event called Sci Foo. Sci Foo is often described as a 'Burning Man for intellectuals' or 'Woodstock of the Mind', and rightly so. In the course of three days, we got to mingle with some of the best minds in a variety of scientific fields but also journalists, inventors, technologists, artists and other fascinating individuals from all horizons. The ethos of the event is

Fabian Renn-Giles
Source: N. Corsini.

Niccolò Corsini
Source: N. Corsini

to facilitate multidisciplinary cross-pollination of ideas in a relaxed environment. We went from trading jokes with Nobel laureates, stories with eminent writers and debates on a variety of topics with Silicon valley gurus without batting an eyelid. For the intellectual ferment of the Renaissance, look no further!

The open format of the event also gave participants the opportunity to show off their latest toys and gadgets. Notable examples included remote controlled cockroaches with neural implants, self-assembling robots, human-powered helicopters and the list goes on. We decided to do our very own demo to illustrate the concept behind CrowdSense and, in the spirit of the TSM-CDT, built a 'human atomistic simulator'. In a nutshell, we mapped the dynamics of a crowd of volunteers using sound and applied concepts borrowed from chemistry to analyse its collective behaviour. In other words, we equated individuals to atoms. A few sleepless nights were spent soldering and coding on the plane and in the hotel room to get it working but it was well worth it. It is hard focusing on writing-up the PhD thesis with such vivid memories at the back of my mind!

Run on Sun

Thomas Edwards shares some insight on the Climate Change Hackathon and on using his skills to help society.

For a while I've been wanting to make a positive difference to the world. That's one of the reasons I applied to the TSM-CDT. My research in modelling solar cells reflects this aspiration.

In pursuit of my social enterprise dreams I took part in Hack4Good 0.6, the planet's biggest ever global hack against climate change. Coders, designers, scientists and entrepreneurs formed teams both locally and internationally to create an app, website or data visualisation over one weekend in September. This competition took place simultaneously in 40+ global cities spanning all continents.

Source: T. Edwards

I packed my sleeping bag and headed to the London competition, upstairs from the New Zealand consulate. We had unlimited supplies of free coffee, tea, food and beer. The space was very wacky and creative, full of half finished hardware projects, random books, a wikihouse and a statue of a cow. People were wandering about from table to table, seeing what other teams were up to and helping out. I think this creative and open format could really benefit academic workspaces!

There were tonnes of great projects at Hack-4good, such as a flooding map, a website for ranking the greenest councils, an open platform for corporate CO_2 disclosure and a dating app for threatened trees.

The project that caught my eye was Friends of the Earth's "Run On Sun" campaign. The idea was to encourage schools to go solar. I joined this team and developed a web tool for calculating the amount of money saved if you install solar panels on your roof. Ordnance Survey data was used to calculate the area of each rooftop, which was subsequently used for the solar potential calculations. We also demonstrated a proof of concept simulation where satellite LiDAR data is used to calculate the shading and slope of each rooftop, resulting in a highly detailed map of solar irradiance.

Our team won gold medal for the London competition and best "Energy and sustainable business" for the global competition. I'm currently working hard to further develop Run On Sun. Recently I went to a solar industry event, "The Big Idea Solar", to pitch in front of venture capitalist dragons. Despite the half completed website and lack of a business model, they really liked the idea and during the break I was inundated with business cards. Afterwards I was even asked to do some research for the Green Party!

Things are starting to get exciting but I could do with a bit of help. If you have a flair for algorithms, python scripting or web development then contact me via the website: *runonsun.co.uk.*

Source: T. Edwards

POSTed to Parliament

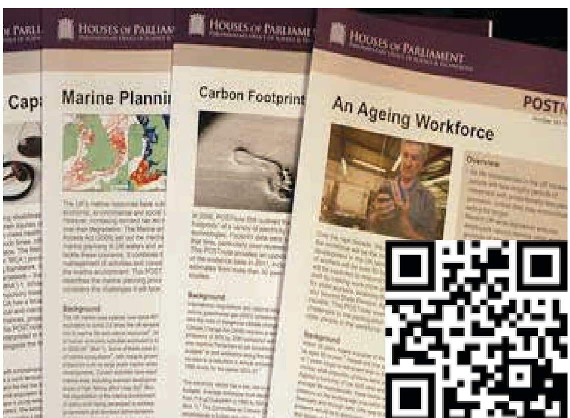
Source: E. Hossinger

Daniel Rathbone *on preparing scientific reports for Members of Parliament as part of his POST placement.*

I recently completed a three-month fellowship at the Parliamentary Office of Science and Technology (POST) funded by EPSRC. POST is an office of both Houses of Parliament tasked with providing impartial four page briefings for parliamentarians on policy issues with a science and technology focus. The topics covered in these briefings or 'POSTnotes' are decided by a board of MPs, peers and outside experts; ensuring that they are timely and of interest to parliamentarians. I was based in offices on Millbank, close to the Palace of Westminster.

During my fellowship I researched and co-wrote a POSTnote on Big Data, Crime and Security. This was part of a series of notes produced as part of an ongoing 'Big Data' theme. Big data is a term used to describe data that cannot be dealt with using traditional analysis techniques (such as spreadsheets). The note covers a number of ways big data held by the police and security services can be exploited to improve policing and security as well as the issues that arise from its use.
Researching the note required interviewing stakeholders from a wide variety of backgrounds including academics, the police, software companies and government departments. Talking to these stakeholders was a very interesting and engaging process and I learnt a great deal about an important and growing area of policing and security. Once the note was drafted it went through a process of internal and external review for accuracy and balance before being published online. As a result of my work at POST I was asked to present my research at a masterclass on big data in policing at the College of Policing, which was a new and exciting experience.

I really enjoyed my time at POST and it was great to see how scientific evidence is used in the work of parliament and the policy making process. It has certainly encouraged me to pursue a career in science policy when I finish my PhD. It was also great to spend three months in parliament learning more about how the legislative process works as well as being able to walk around the Palace of Westminster, attend Prime Minister's Questions and climb Big Ben!



Source: POST

Alumni

This Year's Graduates: Spotlights

David Edmunds

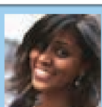
Now applying the analytical skills developed at the CDT to model and visualise risks and side effects in Radiography in a 3 year Post-Doc with NHS Royal Marsden Trust. He felt that the practice in independent research and the computational skills from the CDT have served him well.

When asked what he missed most about the CDT he said, *"The thing I miss most about the CDT is all the people and the great collaborative nature of being part of a large cohort."*

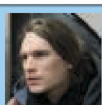
Richard Broadbent

Currently working as a technologist and stress engineer at Rolls-Royce Plc. In his current role he builds model for artificially damaged nickel superalloys in order to predict their fatigue performance.

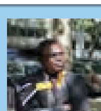
When asked whether the CDT had helped in his role, he said: *"The CDT helped me to meet the people who suggested this job, as well as giving me the invaluable technical skills I use every day in my work."*



Jassel Majevadia
Technical Consultant with IBM

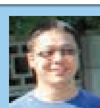


Rob Horton
Post-doc at Imperial



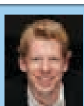
MSc

Ola Olalere
Mechanical Approval Engineer at DNV GL

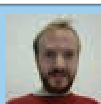


MSc

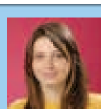
Chenguang Xu
Student at EPFL Lausanne



Aeneas Wiener
Co-Founder of Cytora, an analytic company

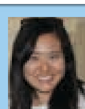


Joe Fallon
Civil Service Operational Research Fast Stream



MSc

Nina Kearsley
Analyst for specialised shipping asset manager

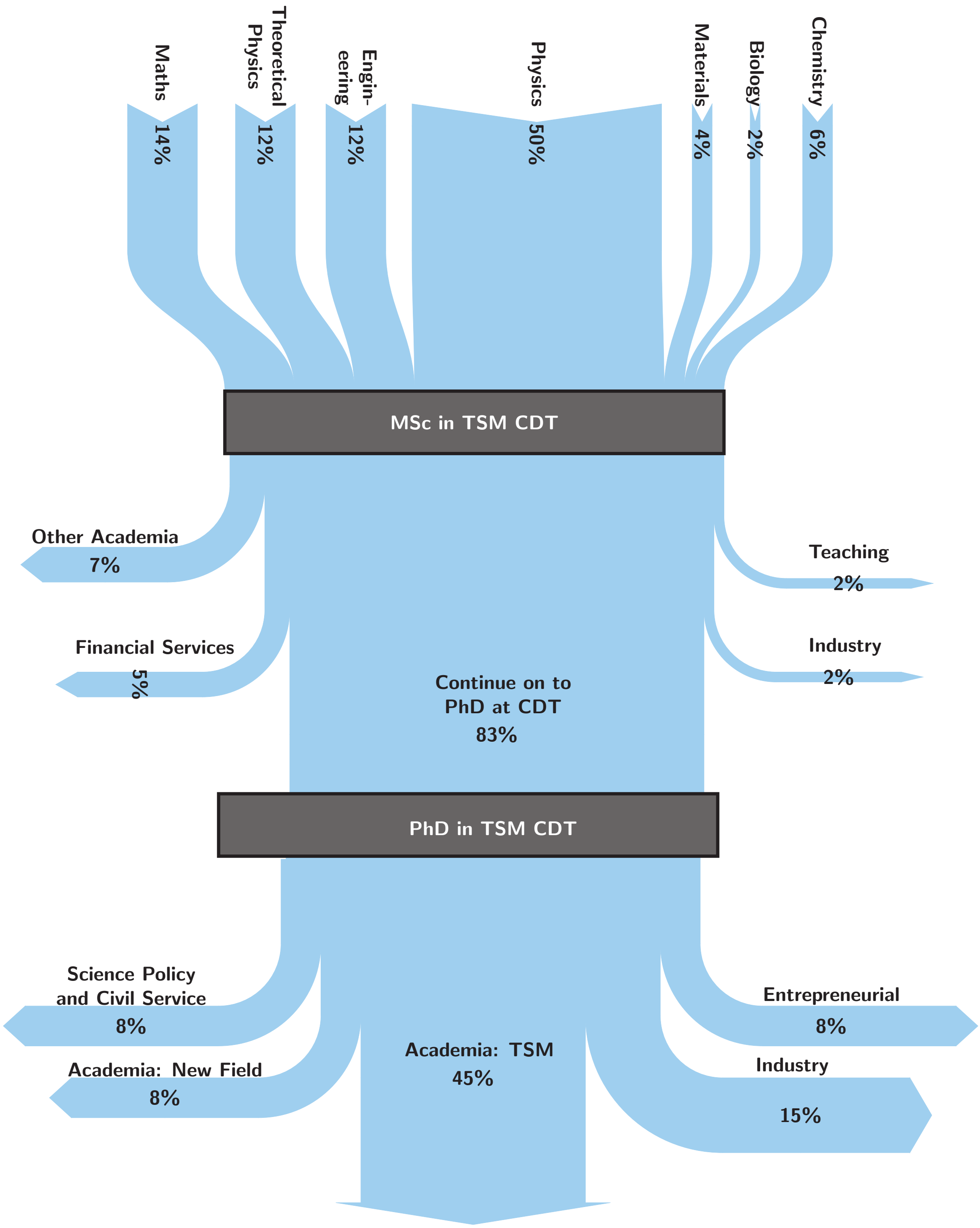


MSc

Jacqueline Tan
Teacher in Singapore

TSM-CDT Graduates: Directions

Where do they come from and where do they go?



TSM-CDT in One Look

Source: sketchfu.com/drawing/85163-so-eye

5th Dec 2008 — TSM-CDT was established by EPSRC

TSM-CDT Begins!

5th Oct 2009 — **Welcome Cohort 1**

5th–9th Apr 2010 — MRS Spring meeting in San Francisco & Master class at Molecular Foundry

16th June 2010 — First International Advisory Board meeting of the TSM-CDT

4th Oct 2010 — **Welcome Cohort 2**

9th May 2011 — Cohort 2 presents a working plane-wave DFT code to Prof. Mike Payne FRS

13th–16th June 2011 — First Authentity course at Cressbrook Hall in partnership with Bloodhound SSC

3rd Oct 2011 — **Welcome Cohort 3**

30th Mar 2012 — First Imperial College CDT Festival of Science

28th–30th May 2012 — First CDT Careers course at Chicheley Hall

27th–30th July 2012 — First student-led Hermes Summer School

1st Oct 2012 — **Welcome Cohort 4**

7th Oct 2013 — **Welcome Cohort 5**

22nd Nov 2013 — EPSRC funds five more cohorts

17th June 2014 — Inaugural TSM Annual Conference

25th–28th July 2014 — Hermes 2014 at Cumberland Lodge

6th Oct 2014 — **Welcome Cohort 6**

Student Publications

Source: F. Ostovari

Classical Mobility of Highly Mobile Crystal Defects. **Swinburne, T.D.;** Dudarev, S.L.; and Sutton, A.P., ***Physical Review Letters***, 113, 215501(2014)

The effect of molecular fluctuations on hole diffusion within dye monolayers. **Vaissier, V.;** Mosconi, E.; Moia, D.; Pastore, M.; and Frost, J.M., ***Chem. Mater.*** 16(16), 4731-4740 (2014)

Optimization algorithm for rate equations with an application to epitaxial graphene. **Posthuma de Boer, J.;** Ford, I.J.; Kantorovich, L.; and Vvedensky, D.D., ***J.Phys.: Condens. Matter*** 26(18), 185008(2014)

Growth of epitaxial graphene: Theory and experiment. Tetlow, H.; **Posthuma de Boer, J.;** Ford,I.J.; Vvedensky, D.D.; Coraux, J.; Kantorovich, L., ***Physic Reports***, 542(3), 195-295(2014)

The reorganization energy of intermolecular hole hopping between dyes anchored to surfaces. Moia, D.; **Vaissier, V.;** Lopez-Duarte, I.; Torres, T.; Nazeeruddin, M.K.; O'Regan, B.C.; Nelson, J.; and Barnes, P.R.F., ***Chem. Sci.,*** 5,281-290(2014)

Interionic Interactions in Conducting Nanoconfinement. **Rochester, C.C.;** Lee, A.A.; Pruessner, G.; and Korneyshev, A. A., ***Chem. Phys.Chem,*** 14(18), 4121-4125(2013)

Collective transport in the discrete Frenkel-Kontorova model. **Swinburne, T.D.**, ***Phys. Rev.*** E 88, 012135 (2013)

New methods for calculating the free energy of charged defects in solid electrolytes **Horton, R.M.**; Haslam, A.J.; Galindo, A.; Jackson, G.; Finnis, M.W. ***J. Phys.: Condens. Matter*** 25, 395001 (2013)

Simulations of nanocrystals under pressure: Combining electronic enthalpy and linear-scaling density-functional theory. **Corsini, N. R. C.**; **Greco, A.**; Hine, N. D. M.; Molteni, C.; and Haynes, P. D. ***J. Chem. Phys.*** 139, 084117 (2013)

Linear-scaling time-dependent density-functional theory in the linear response formalism. **Zuehlsdorff, T.J**.; Hine, N.D. M.; Spencer, J.S.; Harrison, N.M.; Riley, D.J.;Haynes,P.D., ***J.Chem. Phys,*** 139, 064104(2013)

Electron-Energy Loss Study of Nonlocal Effects in Connected Plasmonic Nanoprisms. **Wiener, A.**; Duan, H.; Bosman, M.; Pendry, J.B.; Horsfield, A.P.; Yang, J.K.W.; Maier, S.A.; Fernandez-Dominguez, A.I. ***ACS Nano***, 7, 6287-96 (2013)

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

Awards

Source: Flickr-- Brad.k

Sutton Prize

Mitesh Patel – 2014

Materials Design Graduate Research Prize

Stephen Burrows – 2014

Gabriel Lau – 2013

Materials Design Advanced Graduate Research Prize

Christopher Rochester – 2014

Outreach Prize

Max Boleininger – 2014

Marc Coury – 2013

Major Contribution to the Life of the TSM-CDT Prize

2014:

Organising committee of Hermes 2014

Daniel Rathbone

Thomas Edwards

Benjamin Kaube

Joel Posthuma de Boer

Ali Hammad

Andrea Greco

2013:

Vincent Chen

Musab Khawaja

Daniel Rathbone

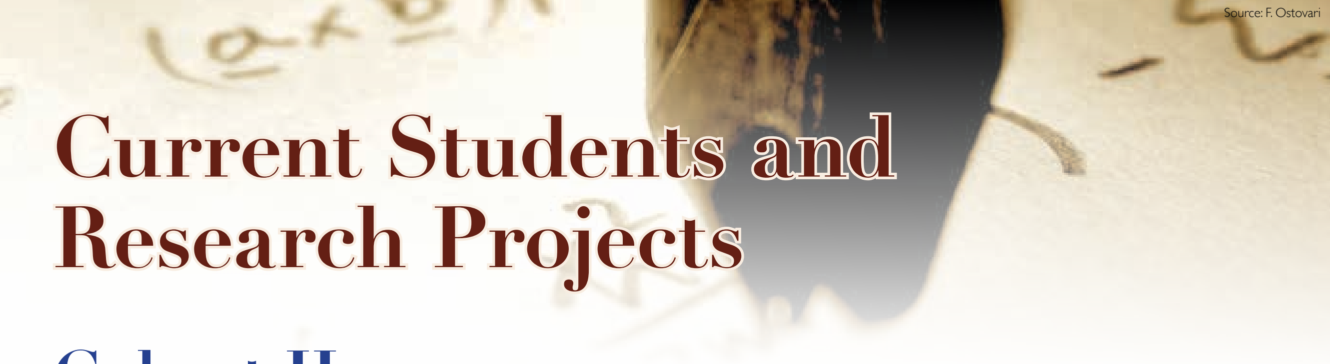
Chiara Liverani

Julian Walsh Prize for Outstanding Contribution to the TSM-CDT:

Marc Coury – 2014

Anthony Lim – 2013

Source: Flickr--Kevin Harber



Current Students and Research Projects

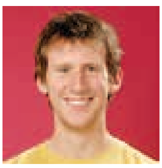
Cohort II

Jawad Alsaei—*Theory and simulation of electronic and optical properties of thin film barium strontium titanate*
Dr Arash Mostofi (Materials/Physics), Dr Paul Tangney (Materials/Physics), Prof. Neil Alford (Materials)

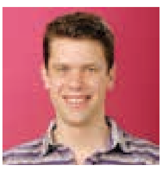
Niccolò Corsini—*Pressure-induced structural transformations in nanomaterials: towards high accuracy large length- and time-scale simulations*
Prof. Peter Haynes (Materials/Physics), Dr Carla Molteni (KCL Physics), Dr Nicholas Hine (Univ. Cambridge Physics)

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)

Anthony Lim—*What excited electrons do*
Prof. Matthew Foulkes (Physics), Dr Andrew Horsfield (Materials)

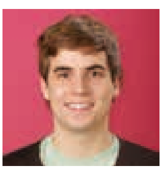


Thomas Poole—*Algorithmic differentiation of quantum Monte Carlo*
Prof. Matthew Foulkes (Physics), Dr James Spencer (Materials/Physics), Prof. Peter Haynes (Materials/Physics)



Fabian Renn-Giles—*Investigating the spatio-temporal dynamics of non-linear dispersive nano-plasmonics with advanced time-domain simulation method*
Prof. Ortwin Hess (Physics), Dr Andrew Horsfield (Materials)

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



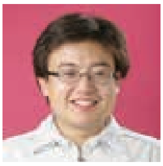
David Trevelyan—*Multiscale simulations of instabilities in complex non-Newtonian fluids*
Dr Tamer Zaki (Mech. Eng.), Dr Daniele Dini (Mech. Eng.), Dr Fernando Bresme (Chemistry)

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)

Valérie Vaissier—*Modelling of interfacial hole hopping in dye sensitised solar cells*
Prof. Jenny Nelson (Physics), Dr Piers Barnes (Physics), Dr James Kirkpatrick (Tessela)

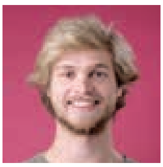
Tim Zuehlsdorff—*Theory and simulation of metal/semiconductor nano-particle interfaces for solar energy storage*
Prof. Peter Haynes (Materials/Physics), Dr James Spencer (Materials/Physics), Prof. Nic Harrison (Chemistry), Prof. Jason Riley (Materials)

Cohort III



Vincent Chen—*Simulation of the solid/liquid interface for Chalcopyrite leaching (with funding from Rio Tinto)*

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



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

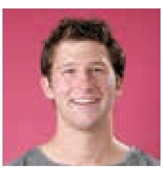
Dr Andrew Horsfield (Materials), Prof. Matthew Foulkes (Physics), Prof. Sergei Dudarev (CCFE), Dr Pui-Wai (Leo) Ma (CCFE)

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

Dr Andrew Horsfield (Materials), Prof. Nic 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)

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)

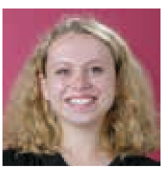
Cohort IV

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*

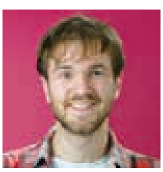
Dr Edo Boek (Chem. Eng.), Dr Fernando Bresme (Chemistry)

Andrea Greco—*Theory and simulation of complex oxide materials (with funding from Argonne National Lab)*
Dr Arash Mostofi (Physics/Materials), Dr Paul Tangney (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*

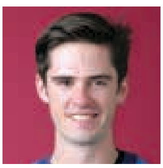
Prof. Mike Finnis (Materials), Prof. Molly Stevens (Materials)

Peter Fox—*Nanoplasmonics and Metamaterials at the classical/quantum boundary*

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

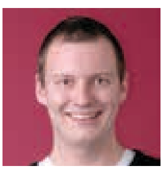
Frederike Jaeger—*Flow of fluids though disordered media with application to membranes: from the molecular to the continuum through the meso-scale*

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)

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), Dr Carla Molteni (KCL)

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—*Theory and simulation of self-assembeled nanoplasmonic metamaterials and devices*
Prof. Alexei Kornishev (Chemistry), Prof. Ortwin Hess (Physics), Prof. Fernando Bresme (Chemistry)

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 (University of Bath), 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 Harrison (Chemistry), Prof. Mike Finnis (Materials/Physics)

Cohort VI – A warm welcome!

Chris Ablitt, Lars Blumenthal, Robert Charlton, Luca Cimbaro (with funding from Rolls-Royce), Jacek Golebiowski, Hikmatyar Hasan, Behnam Najafi, Eduardo Ramos Fernandez (with funding from BP), Iacopo Rovelli (with funding from CCFE), Gleb Siroki, Jonas Verschueren, Alise Virbule, Marise Westbroek.

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