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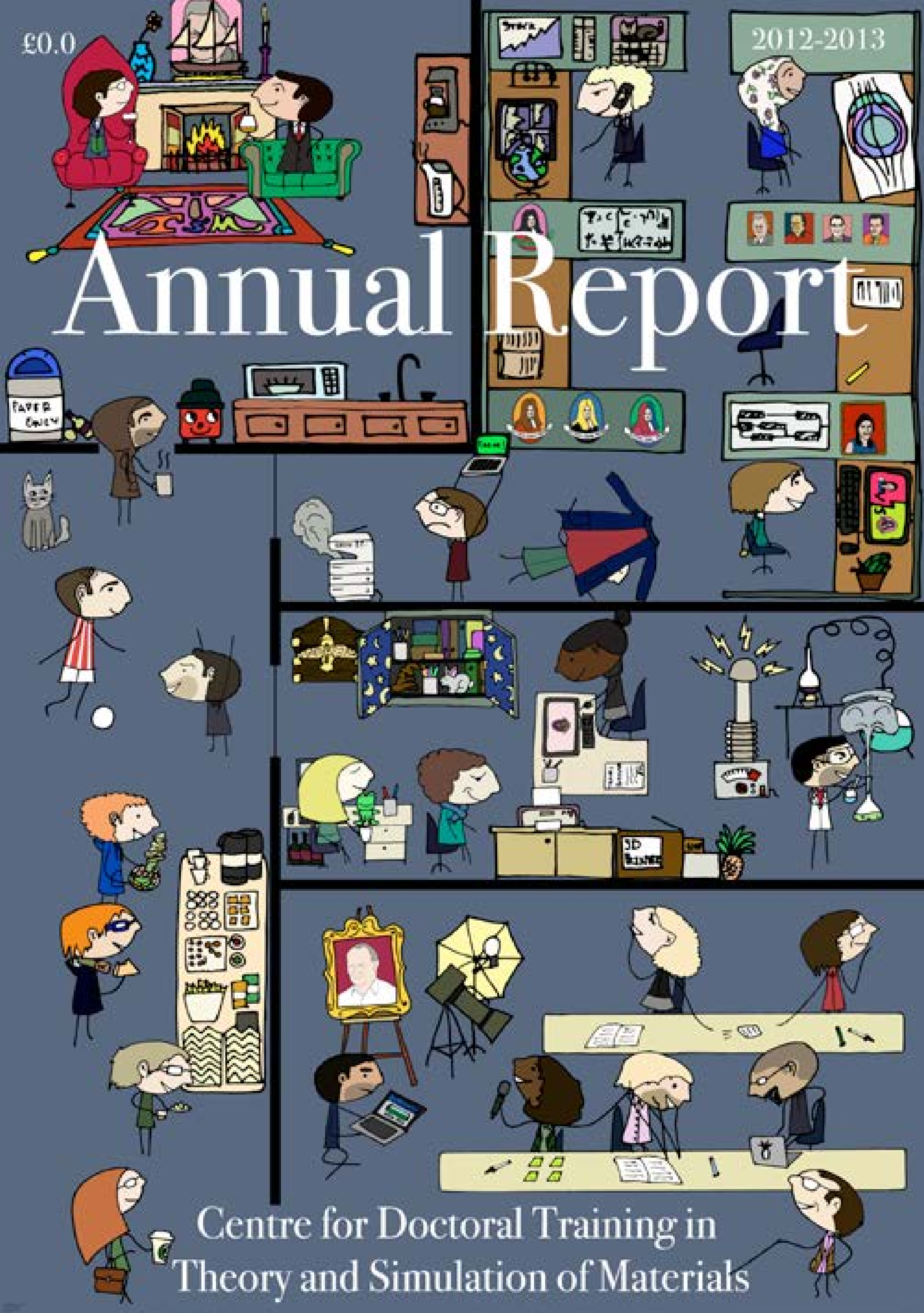
2012-2013

Annual Report



Centre for Doctoral Training in Theory and Simulation of Materials

…In that Empire, the Art of Cartography attained such perfection that the map of a single province occupied the entirety of a city, and the map of the Empire, the entirety of a province. In time, those unconscionable maps no longer satisfied, and the cartographers' guild struck a map of the Empire whose size was that of the Empire, and which coincided point for point with it. The following generations, who were not so fond of the study of cartography as their forebears had been, saw that that vast map was useless, and not without some pitilessness was it, that they delivered it up to the inclemencies of sun and winters. In the deserts of the west, still today, there are tattered ruins of that map, inhabited by animals and beggars; in all the land there is no other relic of the disciplines of Geography.

—JORGE LUIS BORGES, On Exactitude in Science, 1946.

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London, October 2013

Director's Foreword

I AM DELIGHTED to introduce this second annual report of the EPSRC Centre for Doctoral Training in Theory and Simulation of Materials (TSM-CDT). The mission of the TSM-CDT is to create a 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. This report contains our students' own accounts of their activities and achievements during the 2012-13 academic year.

This autumn we have welcomed 15 students into our fifth cohort – a new high for us – bringing to 60 the total number we have admitted to our programmes since the TSM-CDT was established in 2009. At the same time we have begun to say goodbye to members of our first cohort who are submitting their PhD dissertations.

Two trends can be discerned in the growth of the TSM-CDT over the last four years. First, our multidisciplinary MSc course that trains students in TSM across the scales is gaining an international reputation and attracting self-funded students and scholars from overseas, and from Eastern and Southeastern Asia in particular. Second, there has been a significant deepening of our engagement with our industrial partners with co-funding for current students coming from Rolls-Royce, Baker Hughes, Element Six and others.

However the most exciting aspect of this external engagement has been the involvement of prospective employers of our students in the design and delivery of our training. One example of this is our partnership with Materials Design, a global leader in computational materials science and engineering software and services, which has identified our students as potential employees and customers. While we have just welcomed our first Materials Design Scholar into the TSM-CDT, these pages reveal many other aspects of our collaboration. On page 9 you can read about Tom Poole's internship in New Mexico this summer, and there are articles about the winners of the Materials Design Graduate Research Prizes on pages 28 and 29. Staff from Materials Design have also delivered Master Classes, contributed to our Career Planning course and serve on our International Advisory Board.

The ambition of the TSM-CDT is to continue to innovate and improve on the training we deliver, and our deepening relationships with a number of key partners is providing a timely impetus for that. I hope you enjoy reading about more examples in the following pages.

Peter Haynes

In Memoriam
Julian Walsh

The very sudden and wholly unexpected death of Julian Walsh on 23rd September stunned us all. Adrian Sutton paid this tribute at the time: "Julian was a friend and colleague to all of us in the CDT. His boundless energy and enthusiasm inspired and encouraged students and staff alike. When we worked on the proposal for the CDT in 2008 Julian stressed the importance of student leadership and of innovation in professional skills training. His advice was spot on, and his thinking has had a strong influence on the ethos of our CDT. He helped to make Hermes 2012 a great success. He had a vital role in making Authentity, the Ethics courses, the Career Planning course and the Science Communication course happen. He described himself as a 'professional nagger', but it was his dogged determination to make things happen that led to so many of the things that distinguish our CDT. His greatest passion was not the science, although he recognized its crucial importance, but being imaginative and creative in all aspects of the training and guidance students receive. He was a tremendous supporter of our engagement with industry, and he helped to bring about several of our industrial partnerships. Above all, he wanted to ensure the CDT made an impact on the World outside Imperial, an aspiration we all shared with him."

Julian spent 18 years in the oil industry as an international trader in London, Paris and Los Angeles. Hoping to put his deal-making skills to some educational use, he left in 1992 to work with his alma mater, Imperial College and help to devise, implement and guide a series of research-based multi-million pound strategic alliances with industry. He was among the founding team of two successful bio-pharma start-ups; Argenta and iThemba, South Africa's first research-based pharma company focused on HIV/AIDS and TB.

He became involved in the first round of CDT launches, particularly working with the Chemical Biology Centre and the TSM-CDT at Imperial. He was a driving force for industrial engagement in the Thomas Young Centre, the London Centre for Theory and Simulation of Materials. Together with his wife, Carrie, he ran a French wine importing business: the ultimate self-financing lifestyle hobby.

Julian's reach at Imperial was far and wide. But more importantly, he touched all our lives and many of us will miss greatly his friendship, passion and *joie de vivre.*

Contents

Culham Calling

Source: EFDA

Andrea Greco *on how he learned to stop worrying and love nuclear fusion.*

Just a few days before the end of the spring term, Cohort IV had the opportunity to visit the Culham Centre for Fusion Energy (CCFE), the UK's national laboratory for fusion research just outside Oxford.

Students were given a guided tour around the facilities of JET (Joint European Torus) - the world's largest magnetic confinement fusion experiment, where plasma heated to 100 million degrees (hotter than the core of the sun) combines deuterium and tritium to make helium and release lots of energy. JET is part of a roadmap designed to lead to the first working fusion power station within thirty years.

The students attended engaging seminars on the challenging problems related to the design and optimisation of materials which will play a key role in future research in fusion energy. Without the right materials, it will be impossible for the reactors to withstand the high temperatures and radiation damage resulting from fusion.

The visit to Culham highlighted the important materials challenges related to the development of fusion reactors, reinforcing the role of theory and simulation in providing invaluable insight into these problems. Such problems will surely have to be overcome if there is to be a carbon-free energy future.

Two TSM students are currently working closely with Culham on fusion-related materials-modelling projects - Tom Swinburne (Cohort II) and Marc Coury (Cohort III). CCFE is a key partner of the TSM-CDT: Prof Sergei Dudarev (pictured second from right) serves on the Advisory Board.

Back to the Future

As his *PhD draws to a close,* ***Joseph Fallon*** *sat down with* ***Musab Khawaja*** *for a look back on his time in the CDT.*

Q: *You're now in your fourth and final year in the CDT, but where did it all start - how did you end up doing a PhD?*
A: Well, I left deciding exactly what I wanted to do quite late whilst I was an undergraduate. Then I decided I really wanted to do research, and I was just flicking through Physics World and happened to see an advert for this course and so I got in touch with Peter Haynes. When I came for an interview everyone seemed really enthusiastic and it felt like people were doing something new. So I thought, "*oh, I'll give that a go.*" And it involved the sorts of areas I like – electronic structure, statistical mechanics etc. – so it was the right science and it also felt a bit different.

Q: *You decided to forgo the traditional job market and go into academia then?*
A: I had been looking at other careers and becoming some kind of software programmer or doing something related to accountancy or actuarial work, but doing a PhD just seemed more interesting at the time. I wasn't quite ready to let go of Physics really – I wanted to try a few more things out.

Q: *You ended up joining TSM, where the first year is a master's course with a fairly traditional setup in that you take lecture courses and have exams. How did that compare to your undergraduate experience in Physics?*
A: On paper the material looks similar, but it was taught at a higher level and it was all taught very well. It was in small groups so you got to know the lecturers. And I think that's one big advantage of the TSM-CDT – that when you do come to make the decision about what project you do, you've already met the supervisors and you understand more of the jargon, so you make a very informed decision.

Q: *When it came to making that decision towards the end of your first year, what PhD project did you end up choosing and why?*
A: I'm doing a project studying ferroelectric materials, which are an electrical equivalent of a ferromagnet. And what we do is to combine the computational efficiency of simulations based on classical mechanics, with the accuracy of simulation techniques based on quantum mechanics. I picked it because, like I said before, I've always had a bit of a background in electronic structure and statistical mechanics. But also, my supervisors were just really excited about the sort of problems we were looking at. You speak to them when you're looking at different projects and their excitement rubs off.

Q: *What kind of applications do these materials have?*
A: I don't really work on the application side, but ferroelectric materials have a whole host of really good electronic properties for devices, for example, random-access memory in the future could be done through ferroelectric materials.

Q: *Do you think your work will influence these applications down the line?*

A: It may do. My work is just a small stepping stone. But I've been working a lot in understanding what ferroelectrics look like on the atomic scale. And as they try and miniaturise these devices, it's going to be more and more important that we really do have a good understanding of how these things behave on that scale.

Q: *At the start of any PhD project you set out goals. Looking back, to what extent did you achieve what you set out to, or did it shift along the way?*
A: I think you always achieve slightly less than you'd hoped, because you're always very ambitious when you start out. But the major thrust – the major things we were thinking of looking at – we did. But yes, we were quite ambitious when we first thought of the project.

Q: *And overall, how was the PhD experience? Would you recommend it?*
A: Yeah! I enjoyed it. There were definitely times when things didn't work, and you spend months doing the same things over and over again, and you can't work out why it didn't work. And those times are a bit down, but that's the price you pay for working on something original.

Q: *What would you say was the best thing about the CDT and your time here?*
A: I think the best thing is the kind of community you have. So there are always lots of people working on similar things, and you can bounce ideas off of them. And then when you go to conferences you always know a lot of people going. So it's almost like having a science themed holiday with your friends, which is better than it sounds.

Q: *How do you think your experience in the CDT would compare to a more traditional PhD?*
A: The advantage of the CDT is that it's a lot more structured. It's less that they've just put you in a room and expect you to get on with it. There's lots of other things going on. They take care of you.

Q: *What would you say if you could give one piece of advice to prospective CDT students?*
A: I'd say that if you were thinking of doing a PhD, and you think you want to, just go for it. I don't think there's ever a single good reason for doing a PhD, but if you feel that need to do it, definitely go and do it. And the other thing is that whilst you're doing it, make sure you do bits and pieces outside your research. So read up on things that you don't directly work on, or get involved in other things, because they're really rewarding. And when you come back to your research, you're a lot more refreshed.

Q: *What's next for you?*
A: I'm joining the civil service where I'm going to be doing mathematical modelling for them. I'll be creating models to try and forecast things, based on datasets that the government has. So using some of the skills I've developed in the CDT, potentially.

Q: *Was that always the plan?*
A: I didn't really have a plan. But on the CDT we have a careers course where you go along and there are lots of exercises to help you think what you might want to do, and you get to talk to people who work in a wide range of industries. It gives you a good idea of what options are open to you, and this just seemed really exciting.

Q: *Finally, if you had your time again, and knowing what you do now, would you do it all again?*
A: Yes, definitely, and I'd hopefully make fewer mistakes!

Source: MRS

Notes from a Small Island

Max Boleininger *tells us all about Cohort IV's first trip to a materials conference:*

Following the tradition of the annual conference experience, the fourth cohort was faced with several outstanding conferences to choose from. After weeks of deliberation, we decided to pick the International Conference on Materials for Advanced Technologies (ICMAT) in exotic Singapore, over its contenders. With 30 symposia to choose from and about 2500 participants from all across the globe, ICMAT certainly belongs to the heavy-weight league of materials conferences.

Arriving at the weekend just before the official start, the young cohort readily began exploring their surroundings through a haze of time-zone-jumping-induced tiredness. On the following Monday the opening of ICMAT 2013 was celebrated with an enchanting performance by traditional Lion Dancers. From that moment on we were left to our own devices to choose what to attend. Selecting the right talks was especially challenging for us as the lion's share of presentations were on experimental research. While some talks initially left me more puzzled than enlightened, as the conference progressed, I found that my understanding of the experimental side of materials science was improving. One could say that by the end it had bridged the gap between experimental and computational research in my head!

After a day full of intense talks we went out for dinner and were rewarded with a rich culinary experience one is unlikely to find anywhere in London on a budget. Afterwards, the pool on the rooftop of our hotel offered a great opportunity to relax into the night.

For some of us the stay ended after the conference, but others took the opportunity to travel to other far-flung countries such as China, Thailand, Vietnam, and even Italy.

Source: MRS

Communicating Science

***Jassel Majavedia** communicates her thoughts:*

On the weekend of 5th-7th of July, a group of TSM-CDT students attended an unusual course at the magnificent Cumberland Lodge in Windsor Great Park together with postgraduate materials research scientists from all parts of the country. Equipped with professional recording equipment, the attendees were given the task to create a fifteen minute radio feature that would be recorded at the BBC London studios on the last day of the course.

All just fun and games? No. Although the students certainly enjoyed the weekend, the Science Communication course is part of the professional skills training that TSM-CDT students receive. After all, the vision of the CDT is not only to create world-class scientists but also help them to develop a broader skill set. There is no doubt that communication with the media is becoming increasingly important for scientists.

The course would have been hollow without the incredibly talented facilitators. The BBC's very own Gareth Mitchell (presenter of 'Click') introduced the attendees to the basics of radio journalism and went hands-on in helping the students edit and record some radio features. He also organised the course and was there for last-minute tips at Broadcasting House on the final day.

The TV expert was Bob Sternberg who introduced his listeners to important media jargon and the "do"s and "don't"s of TV interviews (for example, never look into the camera!). His practical and approachable nature helped facilitate the recording of a short TV feature which was one of the many exercises that was ultimately there to prepare the attendees for the "real thing".

However, what really made this course stand out was the choice of the organisers to complement the more "practical" elements of Bob's and Gareth's segments with a solid "theoretical" foundation in media communication presented by the third facilitator, Claire Ainsworth. She introduced her listeners to the different aspects of "story-telling" a good media piece and helped them to understand the different players and motives in the media industry. She also went hands-on in helping the researchers with texts about their own research, which is often a daunting task for scientists.

With all of this preparation, the anxiety to go "on-air" on the last day of the course had vanished and the course participants were at ease when the red microphone light in the studio turned on.

Risk

Not just a game of world domination

***Joel Posthuma de Boer** writes about Cohort III's risky Authentity III adventure:*

On April 4th, members of Cohort III joined up with students from two other CDTs from across the country at the impressive Cumberland Lodge in Windsor to participate in Authentity III, in conjunction with Rolls Royce and the land-speed-record-attempt Bloodhound project.

Participants enjoyed a combination of inspiring master classes in how to gain confidence in public speaking and how a successful team operates, as well as team building exercises designed to push them out of their comfort zone. Needless to say these were far from the usual droll exercises that plague early career researchers.

Most excitingly, students working in teams were given one of five problems inspired by the real day-to-day decisions made by engineers, managers and scientists working for Rolls Royce or on the Bloodhound project. This year the problems focused on a number of aspects of risk, and how it affects the decision making process that Rolls Royce and Bloodhound go through.

All groups prepared and delivered excellent presentations and videos to a panel of CDT directors and a Rolls Royce representative, detailing a number of their interesting and thought-provoking ideas. Cohort III left not only with a deeper understanding of how risk affects the workings of large projects, but also a better idea of how to work effectively within a team. Ultimately they gained much more confidence in their ability to communicate their ideas, something that will surely benefit them throughout their careers.

Career Planning II

Judgement day

***With graduation** just a year away, Cohort II headed to Cumberland Lodge once more, this time for a careers course. **Valérie Vaissier** reports:*

On March 26th, Cumberland Lodge played host once more to the second cohort of the TSM-CDT. This time the focus was on bringing us to think about what we want or are able to do with a PhD in Physics in a careers course organised by the Chairman of the CDT, Prof Sutton, with the help of Imperial College's Careers Advisory Service. Making decisions in life is not usually easy, and after having devoted such a long time and so strenuous an effort to our PhDs, the change stepping into the job market and the "real world" poses can be another challenge on its own.

However, thanks to Chairman Sutton's brilliant organisation, not only did we have the privilege of listening to the life stories of quite an exquisite brochette of successful professionals (from a wide variety of industries and academia, including BP, the charity sector, the public sector, think-tanks, the publishing industry, ...) but we had a chance to meet with every one of them in small groups and hassle them as we wished. This gave as an opportunity to get a better idea of what working for different sectors looks like. Thanks to the smaller group talks, we even managed to get some valuable advice from the speakers.

Alongside this, various careers advisors helped us with the more practical aspects of job hunting, such as shaping our own CVs (which, it turns out, one can never get quite right), and they even organised some mock interview sessions, which gave us all some homework to take back with us.

The course was a valuable insight into what to do after our PhD, and we are most thankful for the time and work the organisers put into it.

Source: Mike Licht

Source: Wikimedia Commons

On the Grueness of Emeralds

The Epistemological Disquisitions of Cohort II during Research Ethics III

RANDALL STEVENS *reports on Ethics III, and its reception by the highly dialectical Cohort II.*

THIS TIME, Oxford philosopher extraordinaire and organiser of the Research Ethics III course Marianne Talbot decided to challenge Cohort II's conceptions of knowledge itself. And what she found was an audience ready to take up the gauntlet and fight back in what became the most enthralling and interactive of all the instalments of the Research Ethics course so far.

As a good scion of the analytic school, Marianne took the stance of a proselitistic dogmatist; a stance which not even the most convincing of all the arguments of the Sceptic persuasion – many of which were put forward, most adamantly, by some of the students of Cohort II that took part in this course – could move her from.

The day served both as a routine-breaker and as a brilliant introduction to the most relevant problems of epistemology. Discussions ranged from whether true knowledge is achievable at all or, else, whether scientific knowledge of the world is an illusion; to whether an emerald that is blue until observed green is actually blue, green, grue, bleen or inexistent.

Marianne might not have succeeded in convincing anyone of the truth behind her views but, after all, the aim of this course laid elsewhere. And as an engaging and mind-challenging introduction to the different conceptions of knowledge that there are, Marianne was not only successful, but a pleasure to argue with.

Source: Choco Leibniz Gmbh

CHOCO LEIBNIZ: the best of all possible biscuits

Delectable Leibniz

Is there anything Gottfried Leibniz did not do? From chocolate biscuits to integral calculus, Leibniz contributed to all arts and crafts ever developed by humankind. During the ethics course, a few students did not miss the chance to argue against his claim that "an idea is true, when its notion is possible and false when it includes a contradiction." After all, even nowadays some of the most reputable logicians such as Graham Priest believe in true contradictions.

Tom's Tales

***The first** major collaboration between the TSM-CDT and Materials Design, Inc. was a dream internship: sun, sky, mountains, and a whole load of great science. **Tom Poole** tells us some of his story from the Rockies...*

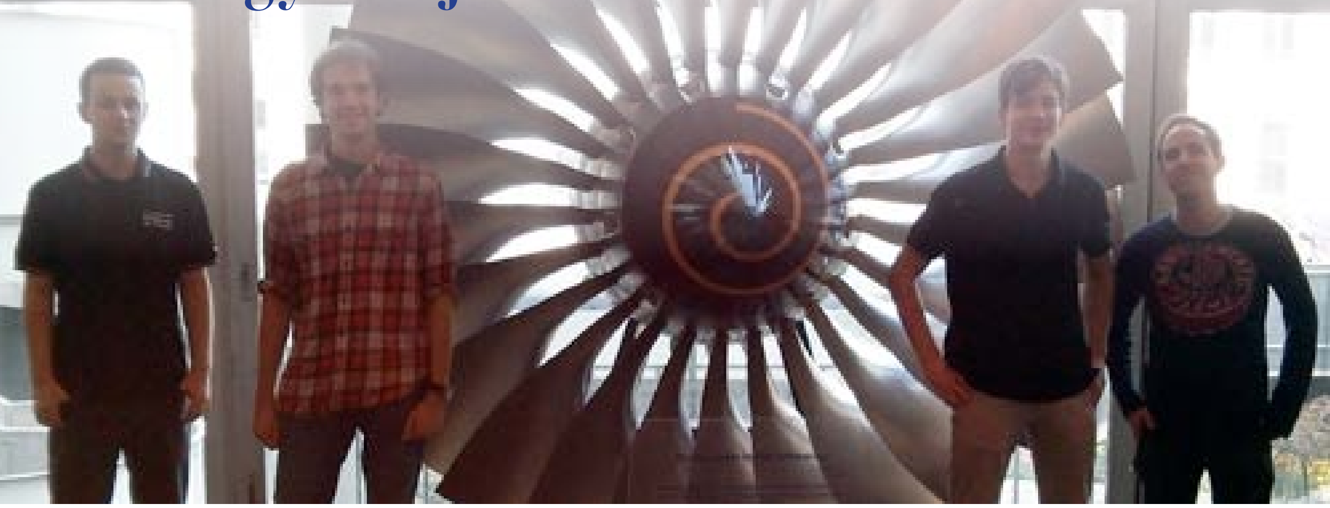
Summer bore witness to the beginnings of a collaboration between the CDT and Materials Design, Inc., a software company that shares the CDT's objective of simulating materials across a range of length and time scales, and whose flagship product, MedeA, provides a unified interface to commonly used, yet disparate, computational tools that support materials science research at Imperial College. On offer was a summer-long internship at the Materials Design headquarters in the skiing village of Angel Fire, New Mexico, nestled in the most southern reaches of the Rocky Mountains. As the most enthusiastic of the potential guinea pigs it fell to myself to take the CDT to new heights (2600 m) and voyage into the realm of corporate academia.

Whilst remaining an unlikely site for such an organisation, northern New Mexico is a surprisingly beautiful part of the country. Here the altitude, and resultant snowfall, paint a very different picture to the typically dusty scenes associated with the state. Sat in a cool, verdant valley I was tasked with creating an intuitive user interface to control the process of molecular dynamics forcefield fitting, an assignment which exposed me to a myriad of computational techniques and many new aspects of materials simulation. Augmenting this influx of practical experience, I also formed part of the Materials Design entourage attending conferences spanning the width of the USA. These events gave me a rare insight into the interaction of industry with academia, as well as providing an avenue into a somewhat unfamiliar scientific community. Whilst the personal benefits of such an opportunity are clear, the internship can be considered a bilateral success as my own technical expertise fed back into the work undertaken over

the summer. With both sides gaining from the enterprise, future CDT students can look forward to similar opportunities presenting themselves in the future.

Buried by Paperwork!

Adam Ready on the Group Research Strategy Project

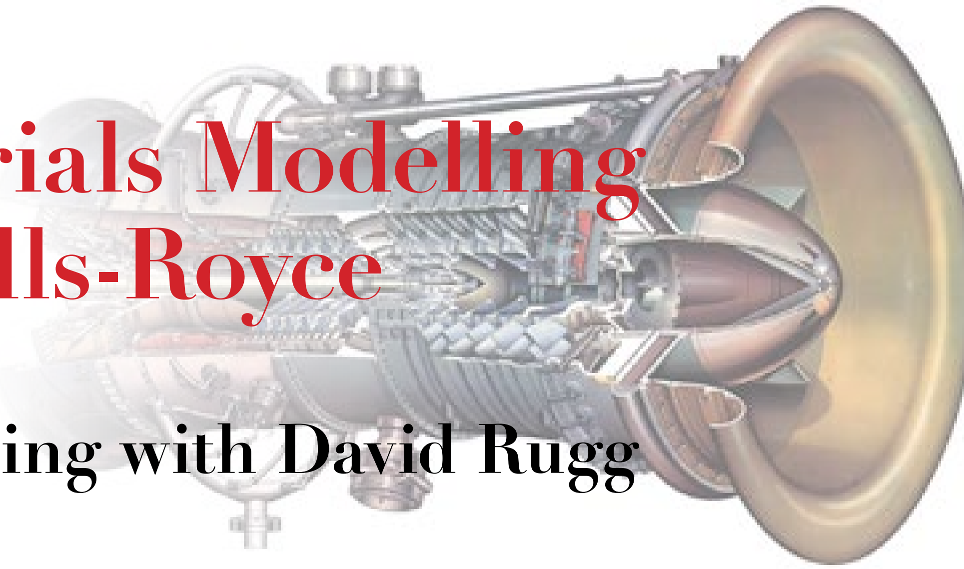


When asked about the day-to-day activities of academic researchers, the writing of grant proposals is not usually the first thing that will spring to mind for most students. However, not only is this a significant part of research, the skills and practices that are brought to bear are often crucial in carrying out the research itself: developing strategies for solving complex problems, collaboration with other researchers, and communicating these strategies in a clear, concise manner.

The motivation behind the Group Research Strategy Project (GRSP), which took place in the spring term of the 2012/13 academic year, was to give the students of Cohort IV an opportunity to develop these skills. This was done by splitting the students into two groups and giving each a different materials problem suggested by industrial partners of the TSM-CDT. The groups each had to write a research proposal detailing a strategy for solving the problem, then present and defend this strategy by answering questions from an interview panel, all in the style of EPSRC's grant assessment procedure.

As one of the two project coordinators my group and I were given a problem by Roll Royce plc. This involved investigating two Titanium alloys in the context of the fatigue failure mechanism known as cold dwell fatigue, a challenging, multi-scale materials problem. To get a good idea of the problem and the methods needed in the investigation we spoke with a number of different experts from disciplines ranging from experimental metallurgy to computational physics. We all found the course to be unique, and the industrial contact intrinsic to the structure of the GRSP gave us a valuable insight into the relationship between scientific research and industry.

Materials Modelling in Rolls-Royce



Source: tcturbines.com

An evening with David Rugg

***Professor David Rugg**, Fellow of Rolls-Royce, delivered a masterclass stressing the relevance materials modelling has to the aersopace industry.*

IF THERE is a strategic sector where materials modelling is the key to success, it is the aerospace industry. Along these lines, on the 16th of January, Prof David Rugg - seemingly the holder of as many job titles as the Grand Poobah - delivered an engaging masterclass where technical details were set aside to stress how materials modelling fits into the greater picture of the aerospace industry.

The performance of jet engine technology, he pointed out, is determined by the turbine entry temperature: the higher, the better. A well guarded secret, having a material able to withstand the pre-determined loads at a few degrees higher than your competitor can make the difference between bankruptcy or success, so companies such as Rolls-Royce devote huge amounts of resources to fine-tune the alloys used and the analysis techniques they employ when designing their engines. Of course, the story does not end there; after all, jet engines are designed to withstand a huge range of highly demanding situations where all its parts, from the fan blades to the casing, must comply.

Prof Rugg then went on to offer a series of examples where modelling techniques such as dislocation dynamics had been employed to inform models used by the jet engine designers, and how it is in many cases thanks to the collaboration between industry and the academic community that the problems arising in the day-to-day engineering practice of aerospace companies can be successfully solved.

After the masterclass, some students had the luck to enjoy Prof Rugg's company over dinner. Despite the black out that forced the restaurant's kitchen to close, the richness of the conversation and the range of topics covered over the table talk offered them a better idea of what working in research for industry looks like.

Source: Oxford Univ. Dept. Materials

Seminar Highlight

With Baker Hughes

***Towards the** end of September, the TYC welcomed **Baker Hughes** for a masterclass on industrial research.*

Baker Hughes is a $20bn per year oilfield services company, which provides the oil and gas industry with the products and services they need to get their valuable hydrocarbons out of the earth. These are typically not easy to extract, and so provide significant materials challenges.

Who could be better placed, therefore, to provide the latest in the TYC masterclass series on "Scientific Careers in Industry"? In attendance were three experts with nearly eighty years of industrial experience between them - Mr John Stevens, Manager of the Materials Center of Excellence at Baker Hughes Texas; Dr Jimmy Eason, Technical Advisor at Baker Hughes Texas and Dr David Curry, Technology Fellow at Baker Hughes UK.

The first session focused on the career paths of the speakers. They described how, despite coming from a variety of academic backgrounds including metallurgy and natural sciences, they very quickly found themselves immersed in industry-based materials research. They explained how although their company fostered an immersive research environment where they were able to "*play*", they ultimately had to be able to justify their work to their shareholders.

Dr Eason then delivered a lecture in which he highlighted the importance of anisotropic limits in materials design. Accounting for anisotropy in finite element simulations is computationally expensive, so an unthinking engineer may be tempted to arbitrarily assume isotropy. The limits for where this might actually be appropriate were derived using some simple yet illuminating models.

This masterclass was the result of what is a burgeoning relationship between the CDT and Baker Hughes, who are sponsoring two TSM students to study the failure of elastomer seals: Nicola Molinari (Cohort V) and Musab Khawaja (Cohort III). Dr David Curry also sits on the Advisory Board and participated in the Careers Course.

Source: Baker Hughes

Source: Imperial ThinkSpace

Entrepreneurship in the CDT

The inception of newsflo

***TSM students Ben Kaube** and **Tom Poole** start up newsflo, providing bespoke media monitoring for academia, charities and government.*

NEWSFLO IS A provider of bespoke media monitoring solutions to universities. Co-founded by two TSM students, the newsflo team consists of seven Imperial College London graduates united by a passion for innovation, science communication and the application of technology to solve real-world problems.

"The technical problem-solving skills fostered by the TSM-CDT left me perfectly equipped for the competitive world of software innovation," says Ben Kaube, TSM student and CEO of newsflo.

Newsflo grew out of the ICStartup+ accelerator programme organised by Imperial Innovations, and in September 2012 received seed capital from Digital Science via their Catalyst Grant programme to support the development of the newsflo platform. Using the Catalyst Grant, newsflo were able to invest in server infrastructure and hire freelance programmers to accelerate the development process out of Imperial College's shiny ThinkSpace offices - a work-space especially designed to nurture start-ups. Working with Digital Science allowed newsflo to learn from their extensive experience on how best to serve the higher education market.

One year later, progress has been exceptional and newsflo are currently negotiating their first contract with a prestigious London university.

For more information, visit
newsflo.net

newsflo
bespoke media monitoring

The Outreach Report
With Simon Foster

Outreach officer Dr Simon Foster *reports on the outreach activities carried out by CDT students in the last year.*

IT HAS been a busy year for outreach in the TSM-CDT, building on the success of the previous year's activities, whilst also undertaking and pursuing new opportunities. Students and staff members have all been involved in a range of outreach activities, with just one of the highlights being invited to host our own science busking stand at the Royal Society Summer Exhibition, where TSM students undertook hands-on demonstrations with visitors, helping the public to understand the work we do.

At the Imperial Fringe events, TSM students have taken part in various events at the College giving talks and undertaking demonstrations with members of the College and the public. Furthermore, TSM students were a key feature of this year's Imperial Festival, with a notable highlight being liquid nitrogen ice cream and the 'cold zone' developed by Marc Coury.

During the Physics Department open days, TSM students gave demonstration talks to audiences of over 150 school students as well as conducting hands-on demonstrations with visitors to the department. The TSM played host to a number of A-level work experience students who got to meet people from all levels of the CDT from PhD students all the way up to senior members of staff, gaining a valuable and insight into the work of the CDT.

A number TSM students have given talks at schools around London, helping to promote the work of the CDT and taking physics as a career path. During the Teacher Training Days, staff and students from the CDT have taken part in several workshops, helping teachers to understand the work the CDT does and how to bring it into the classroom.

At the Big Bang Fair, students from the TSM-CDT teamed up with the Institute of Physics to run a stand undertaking demonstrations with the children visiting the stand. And for 'Research in Motion', TSM students took the outreach tricycle out onto the streets of South Kensington as part of the Royal Borough of Kensington and Chelsea's Celebration of Science.

The Confessions of Jassel

*Following the trail of Augustine of Hippo and Rousseau, **Jassel Majevadia** offers us her very own confessions:*

Source: Wikimedia Commons

I HAVE a confession to make. My name is Jassel Majevadia, and I'm an impostor. Or at least, I think I am. Three times on three separate occasions earlier this year I have encountered this strange phenomenon, both widespread and yet commonly unrecognised: *impostor syndrome.*

Impostor syndrome is when you feel like the only fake in a world of real experts - and that one day, you will get caught. Apart from feeling like it every day throughout my PhD, this cropped up at the BBC, of all places!

I was the lucky recipient of a place at the BBC Academy's Expert Women's day, where I was apparently classed amongst 30 incredibly talented women. Quietly hiding behind a cup of coffee I sat in the lecture room, wondering how on earth I had managed to blag my way in. And then it happened… I was outed. The plenary speaker, Daisy Goodwin, announced an interesting fact. Whilst men happen to be in the media "diary" more often than women, when female experts are asked to contribute or comment to a topic, they a) do not consider themselves to be "expert enough", and b) attribute most of their successes to outside factors. In plain English - they consider themselves to be impostors.

Following this I could sense that I was not the only one in the room sighing with relief. Once this topic was settled, we were put at ease with the help of a brilliant "Women in the BBC" trailer which ended with the faces of the 30 participants

My group began with a radio discussion session, as live, in the style of "Start the Week". Listening to the playbacks of our in depth radio discussions I wasn't entirely sure whether it was really us, or professionals who had stepped in for us. We then went on to film our walking "piece to camera", where we recorded two versions of "explain something complicated in one minute and keep it interesting the whole time".

The third session of the day gave us the opportunity to talk with some of the top dogs themselves in a more intimate setting, which was also broadcast live on the BBC Academy website. Helen Hawken of the Discovery Channel, Jane Garvey of Women's Hour and the BBC's own Andrew Cohen were amongst the panel, offering a few tips on what to do and what not to do when working with the media. But they saved the best until last: our "Now Show" interviews, where we were questioned on niche topics such as how scientists in a field such as materials might collaborate with, say, medical professionals.

To conclude, this first BBC Academy event proved to be an invaluable experience which offered insight into the media that isn't often publicised. The scheme is, in my opinion, a great way to introduce more women into the media. Feeling a lot less like an impostor, this is Jassel Majevadia, signing off for the TSM-CDT news.

Sunshine in Scotland

Source: Wikimedia Commons

Valérie Vaissier reports on the Solar Spark experience, to which she and Tom Edwards contributed, in Scotland this year.

In September, Aberdeen hosted a five-day "Solar Spark" workshop for primary school pupils, timed just before the massive outreach event that is the British Science Festival. Altogether, it was seven days during which pupils, teachers and parents came to meet scientists and to discover the coolest stuff of the year. The TSM-CDT was there.

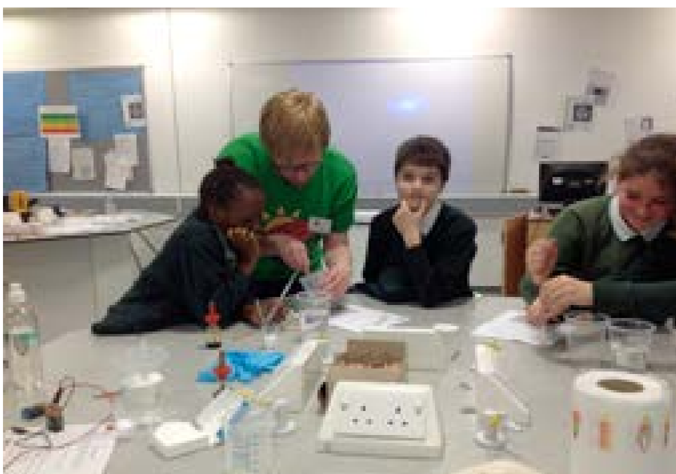
Joining the Solar Spark for the week, we – PhD students working on solar energy – tried to explain the fundamentals of our research. We want to make electricity efficiently using the sun's light. Good. But really, what is energy? What is electricity? What is light?

The Solar Spark workshop consisted of three activities based on these themes. Within an hour, every pupil of a class was given the opportunity to try each activity. As a result, it was a very "hands on" experience and received very positive feedback from pupils and teachers alike.

For the British Science Festival itself, we added activities for older age groups, introducing more complex notions like the principle of energy conversion within a solar cell via a marble run. But the most popular was definitely the "energy slave" experiment. What could you power just by cycling? A microwave? A house?

Find out why you would prefer the sun to do it on the Solar Spark website!

www.thesolarspark.co.uk



Like a Phoenix rising from the ashes

***Fabian Renn** (Cohort II) reports on the mentoring and tutoring scheme for Sixth Form students carried out by a number of TSM students in **The Phoenix High School,** Shepherd's Bush, London.*

In 1994, the Christopher Wren School in White City, London, was one of the most infamous schools in Britain. Listed as one of the eight worst schools in the country, the government decided it needed "special attention". Independent reviewers deemed it so disastrous, it was nearly closed by government on several occasions.

In their despair, the education council turned to Sir William Atkinson—already a successful head teacher at another London school—to take over the Christopher Wren School. Under his leadership, the following four years saw a tremendous improvement in the quality of teaching and student attendance—so much so that the school's name was changed to The Phoenix High School in recognition of the incredible transformation.

In early 2012, the TSM-CDT Chairman Prof Adrian Sutton FRS met Sir William at a public house in the Greater London area. After a brief conversation where Sir William told his story, Chairman Sutton, a passionate advocate for outreach and the importance of science education, was immediately motivated to involve the TSM-CDT in outreach activities at Phoenix.

As a result, in the autumn term of 2012 some students from our CDT visited the Phoenix High School in Shepherd's Bush on Tuesdays or Thursdays, on a weekly basis, to work with small groups of sixth form students on A-level physics. With about four sixth form students per tutor, the sessions were able to be discussion-based problem solving, where the tutor guided the students to the solution of a problem, ensuring that each member of the group understood the answer. This valuable process was facilitated by the proximity in ages between 'teacher' and 'pupil' not often found in the classroom.

Whilst the TSM-CDT students were primarily tutors, they were also an approachable connection to the often aloof and distant world of higher education. Thus, beyond their tutorial roles they also acted as mentors, answering questions such as "How did you get into college?" or "What were your grades?", which allowed the tutors to tell their own stories, often starting in similar places to those of the students, communicating first hand the importance of hard work and dedication. However, the tutors also found that the students were fascinated and motivated to find out more about advanced scientific topics not covered by any curriculum, such as dark matter, entanglement and the Higgs boson.

All the tutors involved found the classes immensely satisfying, and the feedback from the school was extremely positive, with Mr Hider Mahdi, science teacher, reporting "*Last year's mentoring was a great success, the students found the advice and support from your students invaluable.*" Off the back of this initial success, the scheme is being repeated this autumn, coordinated by the TSM-CDT students.

Hermes 2014

The International Materials Modelling Summer School

*After the success of **Hermes 2012**, the summer school-turned-global phenomenon, **Hermes 2014** promises to be at least as good, says one of the organisers,* ***Joel Posthuma de Boer.***

Hermes 2014 is a summer school organised by students from our own Theory and Simulation of Materials CDT, and students of the universities of Cambridge and Edinburgh. It will bring together 50 materials modelling PhD students and early career researchers from around the world, including 15 students on scholarships, giving them the skills to maximise their future impact while promoting teamwork and creating a long-lasting international network.

Students who take part in Hermes 2014 will attend master classes delivered by world leading academics in materials modelling techniques, covering a number of different length scales. These include Craig Carter from MIT, Nicola Marzari from EPFL, Peter Gümbsch from Fraunhofer-IWM and Sharon Glotzer from the University of Michigan. The format of these master classes will be based on the hugely successful Hermes 2012 summer school: after the 60-minute lecture, participants will form groups to discuss the content of the master class before returning to ask the speaker any questions that they have.

In addition, communication professionals will then lead workshops on content and delivery of presentations, including voice and body language skills. Participants will work in groups to produce presentations based on the content of the master classes before getting the chance to speak individually to a small group and receive feedback on their presentation technique. This combination of master classes and communication workshops will help students with the vital skills necessary in science communication for their research to draw the attention of the widest audience possible. They will also become part of an ever-expanding international network of like-minded scientists: the Hermes Academy.

Hermes 2014 will take place on the 25th -28th July 2014 at Cumberland Lodge in Windsor Great Park.

A Feast for Science

***Musab Khawaja** offers us a florid report on the CDT Festival of Science:*

'Twas a crisp spring morning towards the end of March when some 200 students and staff from across Imperial came together for the second annual CDT Festival of Science. The inaugural festival in 2012 had set a high bar, and this year's festival was designed by the student-led organising committee to respond to some of the pressing questions previously proposed, under the banner of "science as a force for change."

The day was kicked off by Sir Peter Knight, President of the Institute of Physics, who explored the role of quantum technology in the 2010 flash crash. Lord Robert May, former President of the Royal Society, continued the fiscal theme in his keynote address, stressing the role of government scientific policy.

The afternoon began with whirlwind tours de force around climate change and drug discovery, by Chris Emmott and Megan Wright respectively. Next came James Clark who brought to life the topic of Green Chemistry, Mike Wright who spoke on Entrepreneurship and Science and the Thomas Young Centre's own Mark Miodownik with his talk, "Stuff Matters."

One of the highlights of the day was the "CDT-off" - a competition between the CDTs consisting of 10 minute pitches from which there could only be one champion. Despite a valiant effort from the TSM trio of Jassel Majevadia, Marc Coury, and Tom Edwards, the Centre for Plastic Electronics emerged victorious.

The day was rounded off by a Question Time-style debate featuring prominent scientists and policy makers including Julian Huppert MP. The audience were able to probe the panel on a range of issues including science funding and immigration; debates that continued long into the evening at the reception...

Research Highlight

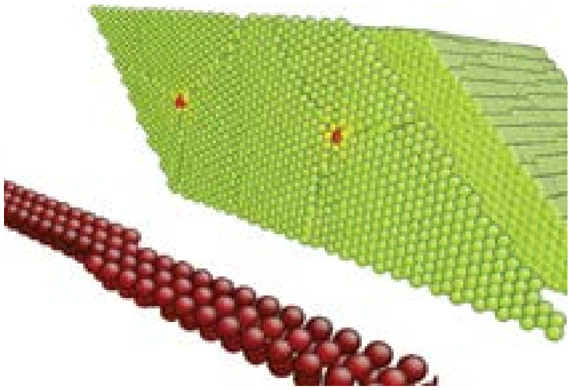
Diffusion of kinks on dislocations in bcc metals

Thomas Swinburne *(Cohort II) introduces us to the topic of his latest paper on kink diffusion in bcc metals, and how some previously assumed ideas about dislocation motion might have to be questioned.*

The highly directional bonding in bcc metals often gives dislocations a non-planar core structure, as a result of which dislocations may move through the nucleation and propagation of double kinks, a process which is completely reliant on thermal activation.

Through this process, microstructural changes often occur under very small (~1MPa) applied stress, on timescales of milliseconds. This is far too slow for molecular dynamics (MD) simulations, which are limited to nanoseconds, but such atomistic methods are essential to understand the dislocation-phonon interaction. To investigate low stress kink-limited motion, we have used a novel simulation geometry to create isolated kinks on dislocations in bcc Iron.

Analytical results for stochastic motion in one dimensional potentials rationalises the wide range of diffusive behaviour exhibited by kinks, from free Brownian motion of kinks on screw dislocations to Arrhenius-law hopping for kinks on edge dislocations. We found the rate of kink momentum dissipation to be temperature independent, at odds with six decades of theoretical work, which states that the rate must increase linearly with temperature due to the increased phonon population.



The kink diffusion simulations are used to parametrise a stochastic line model, the discrete Frenkel-Kontorova-Langevin model. As all length scales are fixed by the crystallographic environment, the model only has three free parameters. This discretisation introduces a new intermediate length scale into plasticity simulation, causing the model to naturally exhibit the wide range of diffusive behaviour seen in MD simulations at around a ten millionth part of the computational cost.

The efficiencies allow access to experimental time and length scales, where good quantitative agreement is seen, giving us confidence to extend the application of this discrete, stochastic model to more complicated dislocation networks.

The publication which forms the subject of this highlight— **T Swinburne**, S Dudarev, S P Fitzgerald, M R Gilbert, and A P Sutton, Physical Review B 87: 064108 (2013)

Research Highlight

Dynamic Dislocation Dynamics for Shock Loading

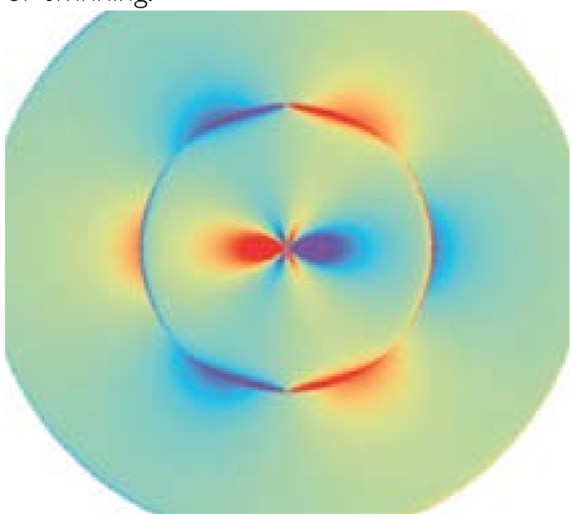
Beñat Gurrutxaga-Lerma *(Cohort II) won the 2012 Materials Design Graduate Research Prize for making dislocation dynamics DYNAMIC (see page 29). Here he discusses his research*

DISLOCATION DYNAMICS is a simulation technique aimed at describing macroscopic plasticity as a result of the collective motions of individual dislocations within an elastic continuum.

Hitherto, dislocation dynamics has mostly been used to answer questions such as why it is that the smaller the size of the sample, the stronger a material seems to be. This applies in situations where the material is loaded so slowly that its behaviour and response can be analysed in a quasi-static, time-independent, manner. Dislocations move in these simulations, but their elastic fields are assumed to be those of static dislocations located at their current positions. However, when quasi-static dislocation dynamics is applied to the study of plastic relaxation in shock fronts, we found it fails in a very fundamental and quite spectacular way: causality was violated. The reason for this was as simple as it was overlooked: the fields of quasi-static dislocations are assumed to propagate instantaneously. If they are coupled with a shock front that propagates at a finite speed - the longitudinal speed of sound - the simulation predicted that dislocations relaxed the material ahead of the front, which violates causality.

Solving this problem meant revamping dislocation dynamics to include time explicitly into simulations of the evolution of the elastic fields. Building on the pioneering work of X Markenscoff and R Clifton more than 30 years ago, we provided a description of the time-dependent fields for the creation and arbitrary motion of edge dislocations that would correct the breach of causality. As a result, interactions between dislocations and between dislocations and the shock front are based on a retardation principle, where the fields take a finite time to propagate.

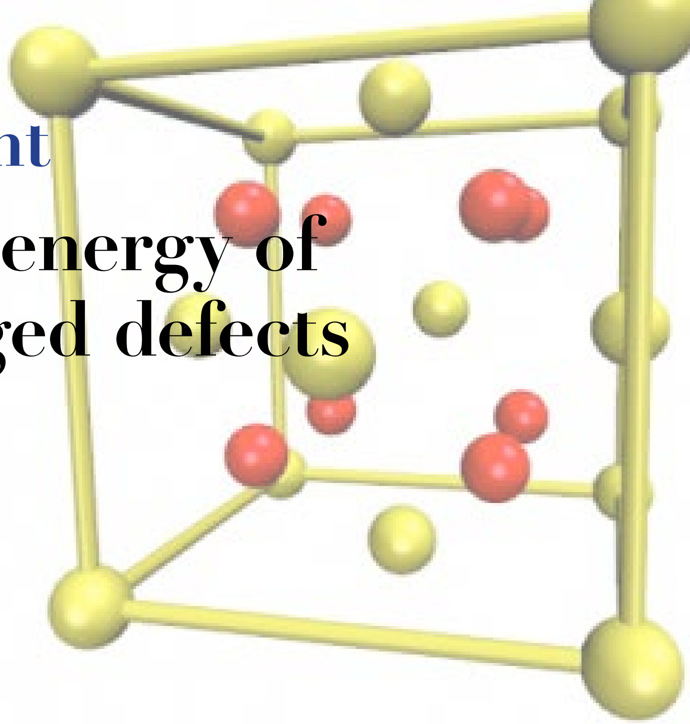
The resulting method, the formulation of which was set out in a recent publication, provides the first truly dynamic formulation of dislocation dynamics. It will enable the study of processes including shock fronts, dynamic fracture, martensitic transformations or twinning.



The publication which forms the subject of this highlight— **B Gurrutxaga-Lerma**, D S Balint, D Dini, D Eakins and A P Sutton, Proc. R. Soc. A. 469: 20130141 (2013)

Research Highlight

Finding the free energy of interacting charged defects



***Robert Horton** (Cohort I) introduces an approach that requires just one calculation for all temperatures with Wang-Landau Monte Carlo.*

THE BEAUTIFUL crystal structures displayed by many compounds are never quite perfect. There are always some missing atoms (vacancies); some impurities also occupy the lattice sites of their host, and sometimes additional atoms (interstitials) squeeze in between atoms of the regular lattice. These defects may be essential to the properties of the material, and the ability to calculate their contribution to the free energy is an important prerequisite for predicting their concentration in real materials. In our work, we introduce an approach for calculating the contribution of charged defects to the configurational free energy of an ionic crystal that may alleviate some of the computational burden of existing methods.

Vacancies in oxides generally carry charge, and repel each other strongly. Mobile vacancies in an oxide carry oxygen through the material and enable solid-oxide fuel cells, and certain gas sensors to work. They are also complicit in the oxidation of metals, which may be bad or good news, depending on whether the oxide is a flaky product of corrosion, or a protective film, as it is on many alloys containing aluminium.

There are numerous calculations in the literature of the energies of isolated charged defects, but the explicit effect of their mutual interactions on the free energy of a material has been neglected, partly because it seems so difficult to calculate. Our article shows how the free energy can be calculated with the Wang–Landau Monte Carlo method. In a single calculation the defects hop around on the lattice and a density of states is generated, from which the free energy at any desired temperature can be obtained easily by one simple integration. We have tested the procedure on a model of point charges representing oxygen vacancies (charge +2|e|) and yttrium ions (charge -|e|) on the cubic zirconia lattice. We found that the free energies could be fitted accurately by a simple regular solution model, with a single temperature-dependent interaction parameter.

Our conclusion is that by implementing more realistic models of the potential energy, such as fitted interatomic potentials, this approach offers a way to incorporate realistic defect–defect interactions in modelling the thermodynamic properties of a range of materials.

The publication which forms the subject of this highlight— **R Horton,** A J Haslam; A Galindo; G Jackson; M W Finnis, J. Phys.: Condens. Matter 25:395001 (2013).

Research Highlight

Hydrogen-enhanced localised plasticity

***Jassel Majevadia** carried out a critical review of the field of Hydrogen Enhanced Localized Plasticity.*

THE DEGRADATION of structural materials by hydrogen-related mechanisms has serious implications for many areas of industry, the most expensive of which is the failure of fuel cladding in pressurised water reactors. The process by which zirconium-based fuel cladding fails is the topic of Jassel's academic research, focussed on the multi-scale modelling of precipitates and delayed hydride cracking in zirconium alloys.

Hydrogen solute atoms have a deleterious effect on the integrity of many transition metals. The consequences of hydrogen related embrittlement range from fuel cladding failure, to everyday items such as fasteners and fixings. Hydrogen embrittlement arises in two ways – environmentally and in the manufacture process. The former is related to failure owing to hydrogen supplied from the environment while the material is in operation, such as corrosion. The latter arises from pre-existing hydrogen within the material that is left over from the manufacturing process.

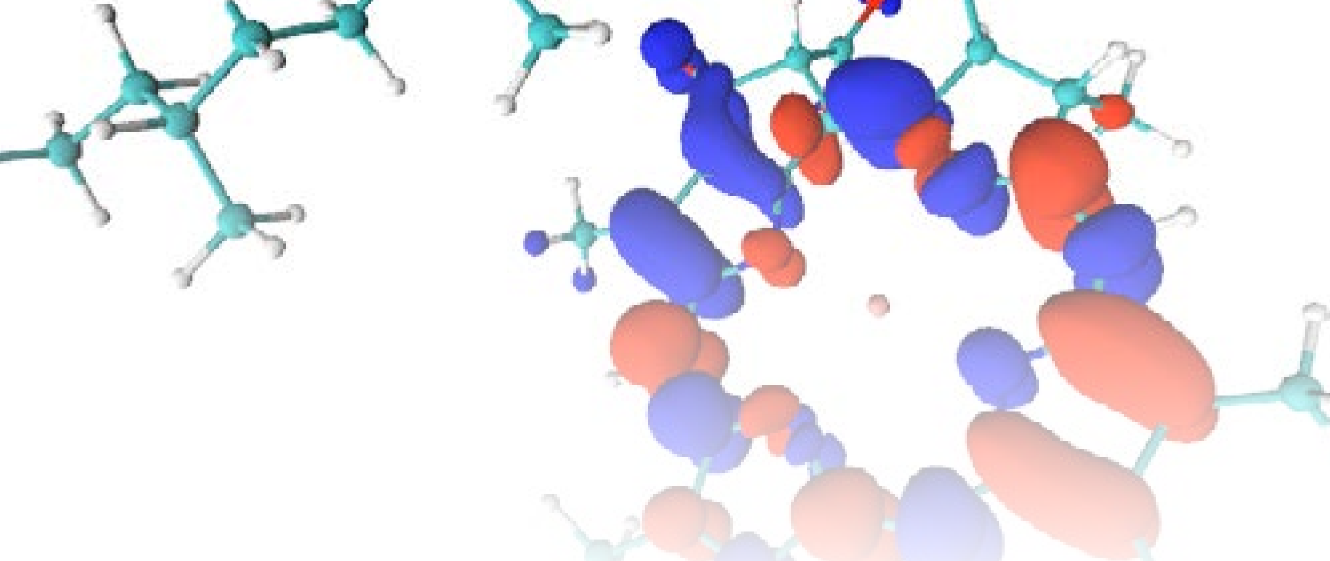
There are a number of proposed mechanisms by which hydrogen embrittles a material, which have varying degrees of experimental support. Researchers in the field of hydrogen embrittlement are currently focusing on three well-known categories: delayed-hydride cracking (DHC), hydrogen-induced decohesion (HID); and hydrogen-enhanced localised plasticity (HELP).

HELP is perhaps one of the most commonly observed mechanisms. Its mechanism was first proposed by C Beachem and is based on the enhanced mobility of dislocations in the presence of solute atoms, leading to lower stresses required to move the dislocations. 'Enhanced mobility' means that the speed of the dislocation is raised for a given applied stress, or that a lower applied shear stress is required to move the dislocation.

The purpose of the article is to review experimental observations and discuss the postulated theoretical models to explain HELP. In addition, further avenues for study that can shed light on both HELP and other observed mechanisms are also outlined.

The nature of hydrogen embrittlement is intrinsically multi-scale, and therefore a fitting topic for a research project within the CDT for the Theory and Simulation of Materials. In particular, Jassel's research aims to incorporate the atomic effects of hydrogen atoms within pure zirconium into continuum models of hydrogen related embrittlement with a view to modelling the accumulation of hydrogen to stress concentrations.

The publication which forms the subject of this highlight— **J Majevadia**, Review: Hydrogen-enhanced localised plasticity–a mechanism for hydrogen embrittlement. Nuclear Future Magazine, 8(3):46-51 (2012).



Research Highlight

Optical Properties of Nanostructured Materials

Tim Zuehlsdorff *(Cohort II) introduces us to his work on faster algorithms aiming at the design of functional materials.*

Over the last 2-3 decades, a substantial amount of research effort in materials science has been focused on developing computational tools to deliver truly predictive models of real life materials. While we are still some steps short of being able to design a new generation of solar cells on the computer, a steady advance in both computational resources and algorithms allows us to address research questions that were impossible to answer only a few years ago.

My research focuses on developing computational algorithms capable of calculating the optical properties of large-scale nanostructures with high accuracy. These nanostructured materials are are of great interest in next generation photovoltaics, since they promise to deliver higher efficiencies than conventional silicon-based solar cells. To capture the effects of the nanostructure on the optical properties of the functional material, large-scale simulations of thousands of atoms are necessary, which are computationally very challenging.

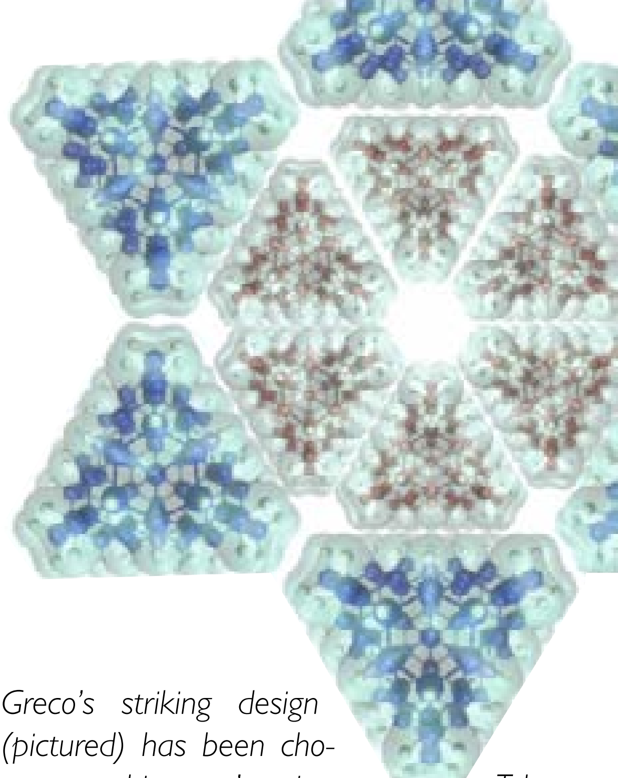
In a recent publication, we developed an algorithm for computing optical spectra that scales linearly with the number of atoms, allowing a treatment of system sizes previously inaccessible.

My work on simulation tools for optical properties is part of the ONETEP code, a simulation software mainly developed at Imperial College, the University of Cambridge and Southampton University for the purpose of modelling realistic large-scale systems. For me, it is very exciting to make my research part of a large software development project, not just because it involves stimulating interactions with a team of researchers at different universities, but also because it allows me to be part of a larger research effort: the ongoing work towards the design of functional materials using computational methods.

The publication which forms the subject of this highlight— **T Zuehlsdorff,** N D M Hine, J S Spencer, N M Harrison, D J Riley, and P D Haynes J. Chem. Phys. 139: 064104 (2013)

What do you get...

when you cross a Christmas tree with a Macintosh?

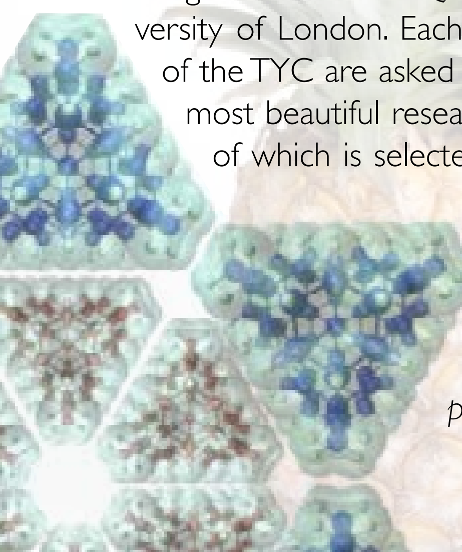


A pineapple! *Congratulations to TSM-CDT student,* ***Andrea Greco*** *(Cohort IV), for winning the annual Thomas Young Centre Christmas card design competition.*

The Thomas Young Centre (TYC) is the London home for theory and simulation of materials, consisting of over 80 research groups at Imperial College London, University College London, King's College London and Queen Mary University of London. Each year members of the TYC are asked to send in their most beautiful research images, one of which is selected as the design for the annual TYC Christmas Card.

'We are delighted to report that Andrea Greco's striking design (pictured) has been chosen as this year's winner. The image is made up of a repeated snowflake pattern of a silicon nanoparticle under hydrostatic pressure. The electronic isosurface (shown in transparent cyan in the image) defines a "quantum volume" for the nanoparticle. This in turn enables the determination of structural phase transformations that occur when pressure is applied.'

The research behind the image was performed in collaboration with Niccolò Corsini (Cohort II) as part of a project on pressure induced structural transformations in nanomaterials, supervised by Professor Peter Haynes, Dr Nicholas Hine (Imperial College London) and Dr Carla Molteni (King's College London).



The publication which forms the subject of this award— **N Corsini**, **A Greco**, N D M Hine, C Molenti, and P D Haynes J. Chem. Phys. 139, 084117 (2013)

Source: Wikimedia Commons

Veni, Vidi, Vici

Student wins award in distant island

He went** there merely intending to explore stranger shores, but buckyball expert **David Edmunds** (Cohort I) ended up winning the Prize for the Best Poster in the MRS - MMM 2012 conference held in October 2012 in the Republic and Island of **Singapore.

Sinbad the Sailor, Zheng He, Magellan and Elcano, Francis Xavier, James Cook, De Bougainville,… all of them famously sailed past the island of Pulau Ujong and the strait of Malacca, off the southernmost tip of the Malay peninsula. David Edmunds, a student of our first cohort, matched their feat on the 14th October when he arrived at Singapore. However, his objective was less exploratory and dangerous than theirs: he was there to present a poster of his research at the MRS Multiscale Materials Modelling conference, that took place between the 15th and 19th October in the Biopolis area of the city.

David has been working on a new approach to the coarse graining of classical molecular dynamics, examining coarse-grained approaches based on the functional integral representation of the dynamics of a system rather than focusing on the equilibrium properties through the partition function. He has been lately trying to apply his approach to a system consisting of a large number of buckminsterfullerene molecules, and presented some of his results in the poster at the conference.

The poster immediately drew the attention of some of the organisers of the conference–he was thoroughly interrogated by Prof Bill Curtin for instance. And, on Friday the 19th, right after the last plenary talk of the conference on the modelling of lobster shells (a topic confusingly appropriate for a conference taking place on island renowned for its seafood and general gastronomic craze), Prof David Srolovitz, chair of the conference, announced that David Edmunds had been awarded the Prize for the Best Poster in the conference. Apart from a diploma and a handshake with Prof Srolovitz, the award included S$250 and the satisfaction of knowing that the poster had beaten the 100 others that were presented in the conference. Let us congratulate David for a well–deserved award!

David is supervised by Prof Matthew Foulkes, Prof Dimitri Vvedensky and Dr Paul Tangney.

Source: Wikimedia Commons

An outstanding prize

for two outstanding people

***Jassel Majevadia** and **Aeneas Wiener** of Cohort 1 have been recognised in this year's Imperial College Student Awards for Outstanding Achievement, established in 2003 for excellence in extramural activity that brings credit to the College.*

Jassel and Aeneas were the principal organisers of the student-led Hermes 2012 summer school that was held at Cumberland Lodge in Windsor Great Park during the London Olympics last July. Designed as "a scientific take on the oldest games in the world", the school attracted students working on materials theory and simulation from across the globe. Far from the traditional format of

a scientific workshop, the event combined master classes from international experts in materials modelling with science communication, challenging participants to convert the content of the master classes into public engagement videos. The vision for this event is clearly explained in the short video on the web site www.hermes2012.org.

The summer school was preceded by an international outreach campaign in partnership with the Royal Society of Chemistry, the RSC-Hermes Ice Challenge, which challenged the public to explain the "Mpemba effect" – why hot water freezes faster than cold. This received over 22,000 submissions from around the world following intense media interest including BBC Radio 4's World at One and Channel 4 News that featured interviews with Jassel and Aeneas. The winning videos and information about the RSC-Hermes Ice Challenge are available online at www.hermes2012.org/ice.

Jassel has continued to develop her skills in science communication, participating in a variety of outreach activities, most recently being selected as the youngest participant at Soapbox Science, an event run by the Zoological Society of London, and L'Oréal Unesco for Women in Science.

Aeneas played a critical role as the first student representative when the TSM-CDT was starting up in 2009-10, and continues to assist with maintenance of the CDT's web site. He has also pursued other outreach activities, including membership of the organizing committee 'Strut our science – fashion show & exhibition with a science twist'. He has also developed a series of online tools introducing TSM to schools: hermesacademy.org/water; participated in a Google mentoring programme; and is Chief Technical Officer for Cytora, a technology start-up focussing on conflict analytics technology.

Source: Cumberland Lodge

Theoretical Kinks at experimental levels

*The Materials Design Advanced Graduate Research Prize for 2013 has been awarded to **Thomas Swinburne** for his research on kink motion of dislocations in BCC metals. His project is supervised by Prof Adrian Sutton from the Department of Physics, and Prof Sergei Dudarev, from the Culham Centre for Fusion Energy.*

Over the last nine months Tom has made outstanding progress including the publication of his first paper in Physical Review B. Tom's impressive and innovative development of a dynamical coarse-grained representation of a dislocation enables kinks to be simulated at experimental stress levels — typically a million times smaller than are accessible to molecular dynamics (MD). Significantly, Tom's work contradicts earlier theoretical analyses but agrees with previous MD simulations. "We have established an approach to model small crystal defect systems, reproducing what is seen in atomistic simulation at a fraction of the computational cost", said Tom and, looking to the future, "the challenge now is to tackle much larger and topologically challenging scenarios in micro-structure evolution, to be in closer comparison with experiment."

Reacting to news of the award, Tom said that he was "very pleased given the quality of the competition!".

Dynamic. Dynamics

***The Materials Design** Graduate Research Prize for 2012 has been awarded to **Beñat Gurrutxaga Lerma** for his work on dislocation mediated plasticity at very high strain rates that is breaking new ground in dislocation dynamics. Beñat is supervised by Professor Adrian Sutton, Dr Daniel Eakins, Dr Daniele Dini and Dr Daniel Balint.*

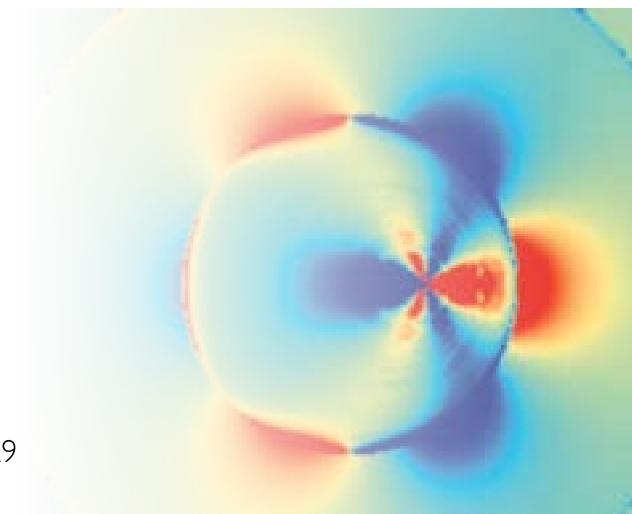
Beñat has exposed a spectacular failure of conventional, quasistatic, dislocation dynamics approaches to model plasticity induced by a shock front as it propagates through an elastic continuum at the speed of sound. In such approaches no account is taken of the finite time required for the stress created by a dislocation nucleated behind a shock front to be transmitted to other parts of the specimen.

As a result dislocation sources are nucleated ahead of the shock front by fields generated instantaneously by dislocations behind the shock front. It is plainly wrong that dislocations are generated ahead of a shock front because no elastic signal can travel faster than the speed of sound. This fundamental failure of all quasistatic approaches to dislocation dynamics rules them out as acceptable methods to simulate shock physics experiments.

Building on the pioneering work of Xanthippi Markenscoff, Beñat has set about the development of a new dislocation dynamics, which solves the time-dependent equations of elasticity. He has derived the time-dependent elastic fields for the creation and annihilation of straight edge dislocations. Together with Markenscoff's time-dependent solutions for the elastic fields of edge dislocations moving at non-uniform velocities these are the fundamental building bricks of a new 2D elastodynamic approach to dislocation dynamics.

Commenting on the most challenging aspect of his research, Beñat says, "The field equations I use offer a closed form solution expressed in the form of the time derivatives of elliptic integrals of the first, second and third kind that are full of singularities. Solving them analytically was out of question, and the numerics have involved quite a lot of tweaking."

He has already shown that with his code he does not see the spurious creation of dislocations ahead of a shock front. He has also developed an ingenious strategy for parallelizing his code in the time domain rather than the space domain. These achievements in just the first nine months of Beñat's PhD are truly outstanding. Beñat himself cites the most satisfying aspect of his work as "the fact that we are pretty much in the dark at the moment: all we know is that we have set foot on shore, and that the land exists. So exciting!"



Busy Bees

***Valérie Vaissier** (Cohort II) and **Marc Coury** (Cohort III) have been awarded the 2012 prize for Outstanding Contribution to the Life of the CDT.*

Dr Tricia Hunt, mentor for Cohort II, praises Valérie, whom she describes as "a strong and unique voice in promoting the CDT and the theory and simulation of materials through outreach. She has helped out at numerous events, including 'science busking' at the Imperial Fringe, Hermes 2012, and a recent teacher-training event in the Imperial College Reach Out Lab. Slightly further afield, she joined a group of students demonstrating solar energy at the British Science Festival in Aberdeen in September 2012, an activity that was organised by a group of researchers based at Edinburgh University who developed a touring demonstration called 'Solar Spark' as part of the EPSRC Supergen programme. Her energy and enthusiasm are further demonstrated by the fact that she is currently planning a very ambitious and wide reaching multi-disciplinary outreach activity with the Natural History Museum".

Tricia continues, "Closer to home, Valérie has also been an outstanding contributor to the life of the CDT by regularly helping with exam invigilation, projects, labs and problem set marking, and is actively involved in the cohort buddy scheme, the CDT Ambassador scheme, and in helping to create new promotional materials for the CDT. What is even more impressive is that she manages all of this at the same time as maintaining an active role in her research group and presenting her research at a number of conferences and workshops."

Cohort III mentor, Dr Daniele Dini, writes about Marc, "Since he joined Cohort III in October 2011, Marc seemed to have been born to be the ideal TSM-CDT student. Always prepared to engage with the (many) CDT initiatives, Marc is the elected student representative of his cohort, and is capable of interacting with both his peers and senior members of staff very effectively. He has demonstrated on many occasions that he is ready to go the extra mile for the the TSM-CDT experience provided for members who are passionate about its credo. In the first few months of his MSc year, Marc acted as glue for his cohort, not only by representing them at Operations Board meetings, but also by coordinating activities and promoting inter- and intra-cohort initiatives."

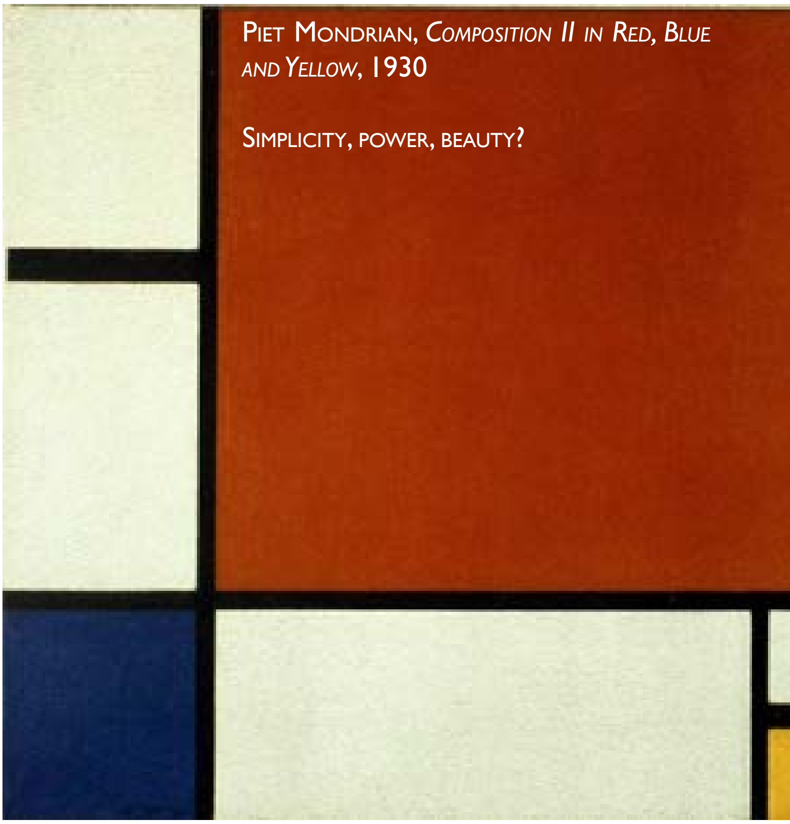
"His other contributions range from being an active attendee and promoter of the TYC, Hermes and other CDT student-led events, coordinating the weekly meetings with the cohort mentor, to organising meetings with other cohorts. Marc helped to finalise the plans for the trip to San Francisco in April 2012 (the trip was arranged for Cohort III to visit the Molecular Foundry at Lawrence Berkeley National Laboratory and to attend the Spring Meeting of the Materials Research Society). He also recently organised a Masterclass with Martyn Sené, interim managing director of the National Physical Laboratory."

Construct, Compute, Visualise?

***Prof Craig Carter** and his research student Rachel Zucker visited the TSM-CDT from 13-15th February and gave a series of workshops on Mathematica. Their aim was to help students "construct models, compute results and visualise them" and they did so by exploring three canonical materials physics problems: the Kronig-Penney model, stability analysis of elastic modes and energy-surface exploration.*

To say that Craig and Rachel fulfilled their brief would be an understatement - they showed how Mathematica really could put the words 'simplicity', 'power' and 'beauty' in the same sentence. Incredibly, no time was wasted on teaching elementary syntax thanks to Craig and Rachel's excellent planning.

To get the competitive juices flowing, the TSM CDT director, Professor Peter Haynes, offered cash prizes for the best Mathematica demonstrations. The five winners were: Musab Khawaja, for his visualisation of spinodal decomposition; Vincent Chen, for his visualisation of the Ising model; Max Boleininger, for his visualisation of solitons; Fabian Renn, for his visualisation of time-varying discrete Fourier transforms; and Anthony Lim, for his visualisation of the tight binding model for Graphene. All winning entries are freely available on the CDT website.



Piet Mondrian, *Composition II in Red, Blue and Yellow*, 1930

Simplicity, power, beauty?

Ruling Rulers

***The TSM-CDT** was delighted to welcome **Dr Martyn Sené** to present a masterclass on measurements, cold fusion and scientific objectivity. **Marc Coury** explains a little bit more...*

'There shall *be but one Measure throughout the Realm*', decreed Henry III in the Magna Carta of 1225, '*One measure of Wine shall be through our Realm, and one measure of Ale, and one measure of Corn, that is to say, the Quarter of London; and one breadth of dyed Cloth, Russets, and Haberjects, that is to say, two Yards within the lists... and it shall be of Weights as it is of Measures.*' This was one of many delightful examples of our need to standardise measurements cited by Dr Martyn Sené, when describing the importance of the work of the National Physical Laboratory.

Champagne by the 125ml glass, cruising at 12 km above sea level. Is this what Henry III had in mind? Source: Airbus

Martyn's own work has spanned the whole range of *technology readiness levels:* in academia he worked on basic technology research before his move to the Harwell Laboratory, and subsequently to AEA Technology, which enabled him to experience the processes by which research is driven up the *technology readiness ladder,* all the way to a viable working new technology. In his current role at NPL, he sits in the middle of this process: between government, academia and business.

Martyn also recounted a fascinating story of his experience with the cold fusion claims of the late '80s. While working at Harwell Laboratory when Pons and Fleischmann famously gave their press announcement in March 1989, he was part of a team tasked with reproducing their results at Harwell. During the summer of 1989, they tried many variants of Pons and Fleischmann's electrolysis cell; but to no avail. At the same time, more press conferences were held elsewhere to announce positive results - although many were later retracted due to the discovery of various mistakes and errors. It was a big deal: cold fusion would have solved many of the world's problems of oil dependency, global warming, radioactive waste, and strip mining for coal. Under pressure from the media, politicians and fellow scientists, Martyn and his team published their negative results in the paper "Upper bounds on 'cold fusion' in electrolytic cells" in Nature in November 1989, which marked the beginning of the end of the cold fusion debate.

Martyn noted some of the lessons learned from his experience with cold fusion, and the importance of trying to maintain scientific objectivity in the face of external pressures such as the media, politics and commerce.

Source: flickr.com

Yes, sir!

***Sir William Atkinson**, executive head teacher of Phoenix High School, visited the TSM CDT on Thursday, May 18th 2013 as part of the TSM CDT masterclass series. **Fabian Renn** (Cohort II) reports.*

Sir William talked about his incredible experience in transforming a deprived London school to an "outstanding" institution as independently rated by OFSTED. In 1994, Phoenix High School - previously known as Christopher Wren School and Hammersmith Comprehensive - was one of the most notorious schools in England. Independent reviewers at the time deemed it so disastrous that it was nearly closed by government on several occasions. Having been listed as one of the eight worst schools in the country, the government decided it needed "special attention".

The education council turned to Sir William - already a highly successful head teacher at another London school - to take over. The following incredible four years of the school's transformation were the focus of Sir William's masterclass: he vividly recalled the ups and downs, the challenges and lessons learned from those four years, sharing his advice from everything on leadership, persistence and motivation.

The masterclass was an immensely inspiring and moving event. Not only was it an amazing opportunity to hear the story of Phoenix High School from the man who turned it around but also to learn about the vision, leadership and staying-power required to make a difference in one of the most deprived areas of the UK.

Sir William Atkinson retains a faint trace of the Jamaican accent that he arrived in the UK with in 1957, aged just seven years old. Thrown straight into a class two years his senior, having never been to school before, he was labelled as stupid. When his real age was finally revealed two years later he had to wait yet another two before he became, what he eagerly says, the only teacher in the country to have failed the 11-plus twice.

Passing through school and managing just a single O-level, it wasn't until he attended sixth form that he finally met a teacher that challenged him. This teacher was the inspiration for his career: and what an extraordinary one it turned out to be. He graduated from King's College London (MA, 1980), and went on to his first headship at the age of 36. Since his inspirational work with The Phoenix, he has also contributed to Channel 4's The Unteachables, and was the inspiration behind Lenny Henry's character in the 1999 BBC television series Hope and Glory.

Source: Accelrys

Accelrys masterclass

***Dr Victor Milman** and **Dr Stephen Todd**, from **Accelrys**, delivered a masterclass on their company's star software product: the materials simulation tool **Materials Studio**.*

RECENT YEARS have witnessed a growing recognition of the importance of software for research. Indeed, software is now viewed as a vital part of the research infrastructure alongside the computer hardware required to run it. Nowhere is this more keenly felt than in computational materials science and engineering, where more and more features are being packed into programs that are required to run efficiently on increasingly complex computer architecture. The task of writing and maintaining such software for global use is no longer a hobby for amateurs, but must combine a professional approach with best practice in software development.

Much of the research in the TSM-CDT inevitably involves the development as well as the application of software for simulating materials. So on 28th November we were delighted to welcome Dr Victor Milman (Senior Fellow) and Dr Stephen Todd (Senior Product Manager) from the Cambridge office of Accelrys to deliver a master class.

Accelrys is a leading provider of scientific innovation lifecycle management software, supporting industries and organisations that rely on scientific innovation to differentiate themselves. This incorporates capabilities in applications for modelling and simulation of materials, collected together into the Materials Studio simulation environment and which include the CASTEP and ONETEP codes for performing first-principles quantum-mechanical simulations with density-functional theory. Indeed two of the authors of ONETEP are none other than Peter Haynes and Arash Mostofi, directors of the TSM-CDT.

Victor and Stephen gave us an insider's view on working in a software company such as Accelrys from two perspectives: marketing and software developer. They explained that a great deal of planning followed up by precise execution has to go into the development cycle of commercial software, and that it involves as much if not more interaction with human beings as with computers. The visit helped us gain a much better appreciation for the software we use in our research, and inspired some of us to think more seriously about a career in the burgeoning software industry after graduation.

Accelrys has supported the TSM-CDT from its earliest days, providing access to Materials Studio to all students within the TSM-CDT. For more information:

www.accelrys.com/products/materials-studio

Student Publications

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)

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)

Rapid Ultrasensitive Single Particle Surface-Enhanced Raman Spectroscopy Using Metallic Nanopores Cecchini, M. P.; **Wiener, A.**; Turek, V. A.; Chon, H.; Lee, S.; Ivanov, A.P.; McComb, D.W.; Choo, J.; Albrecht, T.; Maier, S.A.; Edel, J.B. ***Nano Lett.*** 13 (10), pp 4602–4609 (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. and Haynes, P. D. ***J. Chem. Phys.***, 139, 064104 (2013)

A dynamic discrete dislocation plasticity method for the simulation of plastic relaxation under shock loading. **Gurrutxaga-Lerma, B.**; Balint, D.S.; Dini, D.; Eakins, D.E. and Sutton, A.P. ***Proc. R. Soc. A.*** 469, 20130141 (2013)

Surface Plasmons and Nonlocality: A Simple Model. Luo, Y.; Fernandez-Dominguez, A. I.; **Wiener, A.**; Maier, S.A.; Pendry, J. B. ***Phys. Rev. Lett.*** 111, 093901 (2013)

Influence of polar medium on the reorganization energy of charge transfer between dyes in a dye sensitized film. **Vaissier, V.**; Barnes, P.; Kirkpatrick, J. and Nelson, J. ***Phys. Chem. Chem. Phys.***, 15, 4804-14 (2013)

Theory and simulation of the diffusion of kinks on dislocations in bcc metals. **Swinburne, T. D.**; Dudarev, S. L.; Fitzgerald, S. P.; Gilbert, M. R. and Sutton, A. P. ***Phys. Rev. B***, 87, 064108 (2013)

Review: Hydrogen-enhanced localised plasticity–a mechanism for hydrogen embrittlement. **Majevadia, J.** *Nuclear Future Magazine*, 8, 46-51 (2012)

Nonlocal Effects in the Nanofocusing Performance of Plasmonic Tips. **Wiener, A.**; Fernández-Domínguez, A. I.; Horsfield, A. P.; Pendry, J. B.; Maier, S. A. ***Nano Letters***, 12, 3308–3314 (2012)

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

Current Students and Research Projects

Cohort I

Richard Broadbent—*A Model for Polymer Membranes*

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

David Edmunds—*Course Grained 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 Paul Tangney (Materials/Physics), Dr Arash Mostofi (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 II

Anthony Lim—*What excited electrons do*

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

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)

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

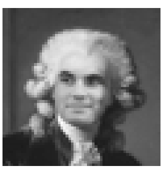
Beñat Gurrutxaga–Lerma—*Theory and simulation of elastoplasticity at very high strain rates*
Dr Daniel Balint (Mech. Eng.), Dr Daniele Dini (Mech. Eng.), Dr Daniel Eakins (Physics), Prof Adrian Sutton (Physics)

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

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), 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 (Chemistry),
Dr James Kirkpatrick (Tessela)

Cohort III

Vincent Chen—*Simulation of the solid/liquid interface for Chalcopyrite leaching*
Dr Patricia Hunt (Chemistry), Prof Nic Harrison (Chemistry), with funding from Rio Tinto

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—*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)

Musab Khawaja—*Towards a Predictive Model of Elastomer Seals*

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*

Dr Andrew Horsfield (Materials), Prof Jonathan Marangos (Physics), Prof Peter Haynes (Physics/Materials), Dr Ruth Pachter (US AFRL)

Stephen Burrows—*Simulation of multiphase electrokinetic fluids: from atomistic to Lattice-Boltzmann methods*
Dr Edo Boek (Chem. Eng.), Dr Fernando Bresme (Chemistry), Dr Xuesong Li (Shell)

Gil-Arnaud Coche—*Multiscale modelling of flow in porous media*

Prof Dimitri Vvedensky (Physics), Prof Peter King (Earth Science & Engineering)

Andrea Greco—*Theory and simulation of complex oxide materials*

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?*
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*
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 – A warm welcome!

Amanda Díez, Peter Fox, Frederike Jaeger, Christopher Knight, Andrew McMahon, Nicola Molinari†, Vadim Nemytov‡, Premyuda Ontawong, Farnaz Ostovari, Mitesh Patel, Andrew Pearce, Elisabeth Rice, Jacqueline Tan, Markus Tautschnig, Chenguang Xu

†Baker Hughes Funding ‡Materials Design Scholar

Alumni News

Ola Olalere (MSc 2010) is working as a Consultant Engineer in the Asset Integrity Team of Petrofac.
Frank Buijnsters (MSc 2011), after having passed the MSc in TSM with distinction, is now pursuing a PhD at Radboud University of Nijmegen on the theory and simulation of magnetic systems under the supervision of Prof Katsnelson.
Nina Kearsey (MSc 2011) is now master and commander of a fleet of ships in the Ocean Sea.
Karlis Kramens (MSc 2012) is now working at Cisco Systems optimising video compression algorithms and code.

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Prof W Craig Carter – MIT, USA
Dr David Curry – Baker Hughes
Prof Sergei Dudarev – Culham Centre for Fusion Energy, UK
Dr Claire Hinchliffe – Sheffield-Manchester AMS-CDT, UK
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Prof Adrian Sutton FRS – Chairman
Dr Arash Mostofi – Assistant Director/Cohorts Mentor: Cohorts I&IV
Dr Patricia Hunt – Cohort Mentor: Cohort II
Dr Daniele Dini – Cohort Mentor: Cohort III
Dr Daniel Balint – Cohort Mentor: Cohort V
Dr Simon Foster – Outreach Officer
Ms Lilian Wanjohi – Board Secretary

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Prof Ferri Aliabadi *(Aeronautics) – Research Board*
Prof Neil Alford FREng *(Materials) – Research Board*
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Dr Pedro Baiz Villafranca *(Aeronautics)*
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Dr Bamber Blackman *(Mechanical Engineering)*
Dr Edo Boek *(Chemical Engineering)*
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Dr Finn Giuliani *(Materials)*
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Prof Nic Harrison *(Chemistry)*
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Dr Jerry Heng *(Chemical Engineering)*
Prof Ortwin Hess *(Physics)*
Dr Sandrine Heutz *(Materials)*
Prof David Heyes *(Mechanical Engineering)*
Dr Andrew Horsfield *(Materials)*
Dr Patricia Hunt *(Chemistry) – Second Cohort Mentor*

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Prof Omar Matar *(Chemical Engineering)*
Dr Michelle Moram *(Materials)*
Dr Arash Mostofi *(Materials and Physics) – Deputy Director and Mentor to Cohort 1&4*
Prof Erich Müller *(Chemical Engineering)*
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Prof Kamran Nikbin *(Mechanical Engineering)*
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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)*
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Dr Carla Molteni *(King's College London)*
Prof Tony Paxton *(King's College London)*
Prof Alex Shluger *(University College London)*
Prof Neal Skipper *(University College London)*
Prof Mark van Schilfgaarde *(King's College London)*

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Mr Piero Vitelli *(Island 41)*
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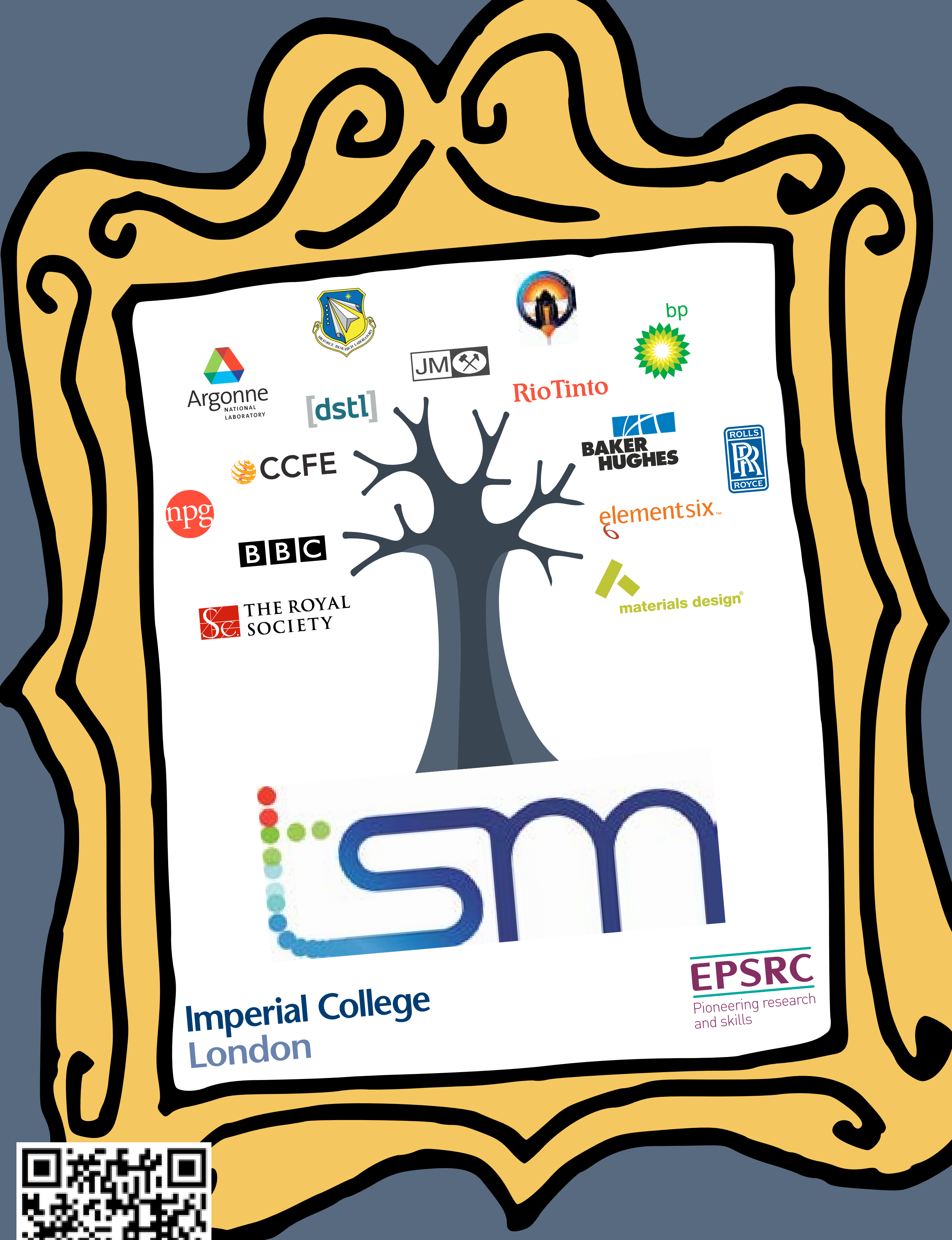
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