

Rethinking the PhD

Adrian P Sutton

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The Author

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Also by Adrian P Sutton

Electronic structure of materials

Interfaces in crystalline materials,
co-authored with R W Balluffi

Physics of elasticity and crystal defects

List of abbreviations

ACM Advanced Characterisation of Materials

AIST The National Institute of Advanced Industrial Science and Technology (in Japan)

BBC British Broadcasting Corporation

CASTEP Materials modelling code based on a quantum mechanical description of electrons and nuclei.

CCFE Culham Centre for Fusion Energy

CDT Centre for Doctoral Training

CEA Commissariat à l'énergie atomique et aux énergies alternatives (Alternative Energies and Atomic Energy Commission in France)

CECAM Centre Européen de Calcul Atomique et Moléculaire (European Centre for Atomic and Molecular Calculations)

CNRS Centre National de la Recherche Scientifique (National Center for Scientific Research, France)

CS Case Study

EOARD European Office of Aerospace Research and Development

EPFL Ecole Polytechnique Fédérale de Lausanne

EPSRC Engineering and Physical Sciences Research Council

ETH Eidgenössische Technische Hochschule (Swiss Federal Institute of Technology in Zurich)

GPP Group Programming ProjectGRSP} Group Research Strategy Project

HEFCE Higher Education Funding Council for England

IAB International Advisory Board

KCL King's College London

MIT Massachusetts Institute of Technology

MML Materials Modelling Laboratory

MPIE Max Planck Institut für Eisenforschung GmbH (Max Planck Institute for Iron Research, in Düsseldorf, Germany)

ONERA Office National d'Etudes et de Recherches Aérospatiales
(French national aerospace research centre)

ONETEP Linear-scaling density functional theory software package

Penn University of Pennsylvania

QMUL Queen Mary University of London

RR Rolls-Royce plc

RSC Royal Society of Chemistry

TSM Theory and Simulation of Materials

TSM-CDT Centre for Doctoral Training on Theory and Simulation of
Materials

TYC Thomas Young Centre

UCL University College London

UCLA University of California Los Angeles

UKAEA United Kingdom Atomic Energy Authority

USAFRL United States Air Force Research Laboratory

Preface

This book is about a Centre for Doctoral Training (CDT) at Imperial College London. Its theme is Theory and Simulation of Materials (TSM) and I was its founding director in 2009.

I am aware that others running PhD programmes have put a lot of creative thought into the PhD experience for their students. I have written this book to put forward ideas we have developed in our CDT. Many of these ideas may be transferable to other areas of science and engineering. I have also included sections more specific to TSM, such as coursework, and the **headings for those sections are in round brackets** so that readers less interested in TSM can skip over them.

I hope this book will be of interest to anyone wishing to set up a centre for doctoral training; anyone having responsibility for doctoral training at either institutional or departmental levels; any undergraduate thinking about doing a PhD; anyone in industry considering sponsorship of PhD researchers; anyone supervising PhD students; anyone involved in the design and delivery of professional skills training in universities; any funding agencies and policy makers thinking about the outcomes they want from PhD education and training.

To distinguish our CDT from other CDTs I refer to it as the TSM-CDT or ‘our CDT’. The TSM-CDT was the realisation of a dream I nurtured since I completed my own PhD in 1980 at The University of Pennsylvania (Penn). The feedback we have received from our funder the Engineering and Physical Sciences Research Council (EPSRC), from our International Advisory Board (IAB), from our industrial collaborators, from academic colleagues in the UK and overseas and from our students is that our CDT is outstanding for its research, education and training, its engagement with the world outside Imperial College and the quality of the student experience.

The ‘we’ in this book is not the ‘royal we’. It refers to Professor Arash Mostofi, who has been the director of our CDT since 2016, Professor Peter Haynes, who was the director between 2011 and 2016, and me as the founding director between 2009 and 2011. From 2016 it also includes Dr Johannes Lischner, who was deputy director. The passion, commitment and leadership of Peter and Arash were essential to the success of our CDT. Arash and Peter read an earlier draft of the entire book and provided many helpful comments and corrections. All remaining errors are my responsibility alone.

Many academics at Imperial and elsewhere in the Thomas Young Centre (TYC) contributed to the success of our CDT. I want to thank particularly those who served as cohort mentors and those who taught in the MSc. Our CDT enjoyed wonderful collaborations with industrial partners. I particularly wish to thank Professor Dave Rugg at Rolls-Royce who gave so much of his time and energy to our CDT. One of the principal reasons for the success of our CDT was the strong engagement and support we received from our IAB. Although it met only once a year its members had a profound influence on how the CDT developed. I would particularly like to thank Professor Craig Carter from MIT who served on the board since the inception of our CDT in 2009 and who came to every one of our biennial Hermes conferences.

We were very fortunate to have superb administrative support staff in Lilian Wanjohi, Miranda Toora (née Smith), Veena Dhulipala and Naho Ollason. Dr Nic Harrigan and Dr Simon Foster provided brilliant training for our students in outreach and public engagement.

Imperial College was the ideal home for the TSM-CDT, not least because it has so many highly talented scientists and engineers looking for a way to work together. I doubt very much the TSM-CDT could have been more successful anywhere else in the UK. I am particularly grateful to the Departments of Physics and Materials for their support of our CDT.

Finally a big thank you to my wife Pat for the title of the book and for reading an earlier draft and making many clever suggestions and improvements.

London and Oxford

January 2020

1. Introduction

1.1 Recent history of the PhD in the UK

The traditional picture of a PhD in the UK is of a lone researcher working independently for three years, under the guidance of an established academic, to make an original contribution to knowledge. It used to be a rite of passage to an academic career. But with 23,650 doctorates awarded in the UK in 2016/17¹, that is no longer possible, although a PhD has become a standard requirement for an academic appointment.

The traditional model of the PhD received considerable criticism during the 1990s (e.g. see Noble (1994)², Wellington et al. (2005)³ and Radon and Sung (2009)⁴), including poor supervision, gender discrimination, low quality of research, poor completion rates, extended completion times and low quality of writing in PhD theses. The traditional PhD has also been criticised for being overly specialised, with little preparation for employment in areas such as working with people. Another criticism is that the traditional PhD was too geared to producing future academics. Some of these criticisms are consistent with my own experience. In the early 1980s the Careers Service at Oxford University advised me to hide my PhD from prospective employers to enhance my chances of getting a job!

Since the Roberts report⁵ of 2002 it has been mandatory in UK universities that PhD students undertake at least 2 weeks a year of training in ‘transferable skills’ - working in teams, communication

¹ <https://tinyurl.com/y926fg89>

² Noble, K. A. (1994) *Changing Doctoral Degrees: An International Perspective*, Buckingham: Society for Research into Higher Education and Open University Press

³ <https://dx.doi.org/10.4135/9781849209977>

⁴ <https://tinyurl.com/scjam5e>

⁵ <https://tinyurl.com/v65s4nd>

skills, public engagement skills, business awareness, entrepreneurship and so on. I prefer the term ‘professional’ skills to ‘transferable’ skills. The research skills acquired during a PhD are also transferable to other career paths. But Roberts did not mean research skills when he wrote about transferable skills. He was talking about the skills required to work effectively with people in a range of professional environments both outside and inside academia. I will use the term ‘professional skills’.

The 4-year ‘New Route PhD’⁶ has a format similar to that of the North American PhD, with taught elements in the first year followed by 3 years of research. The taught elements include training in research and advanced disciplinary study. After a successful HEFCE-funded pilot which began in 2000 in ten universities, the New Route PhD was made available across the UK. The aim was originally to create a UK doctorate that had more appeal to international students, particularly those who might otherwise find it attractive to study for a PhD in North America.

With the added ingredient of professional skills training the New Route PhD was the model on which the CDTs, introduced by EPSRC, were based. Initially these centres were introduced to facilitate interdisciplinary research, such as the interface between life and physical sciences and complexity science. In 2009 EPSRC funded 50 CDTs across its entire remit.

1.2 What is Theory and Simulation of Materials (TSM)?

Over the last thirty years TSM⁷ has become one of the central pillars of materials science. For the reader unfamiliar with materials science I

⁶ see Park (2005). <https://tinyurl.com/qru8uf6>

⁷ ‘Materials modelling’ is an older name for TSM. It is still used widely, especially in industry.

offer a brief introduction⁸. It is difficult to think of any technology that does not ultimately rely on the availability of suitable materials. Literally everything we do every second of every day involves the use of materials, even when we are asleep. Some materials we depend upon absolutely to keep us safe, such as when we fly, or construct a tall building, or put a stent into an artery. Others enable us to carry libraries of books and music in our pockets and talk to people on the other side of the World. The progress of civilisation has been defined by the materials we use, from the stone age to the bronze age to the iron age and now the silicon age.

In the absence of theory and simulation the improvement of existing materials and the development of new materials is entirely empirical. This is indeed how skilful engineers have created most materials. But sometimes this approach is too expensive, or the properties of a material degrade inexplicably in service. There are also occasions when a material is placed in a hostile environment, such as a nuclear reactor, for a period of time far too long to test its performance experimentally. Being able to model the behaviour of the material under those conditions is then the only source of information. Regulators require that a serious failure of a material critical for safety, such as a component in a jet engine, is understood fully and that often requires theory and simulation in conjunction with experimental investigations. These examples illustrate when simulations based on a theoretical

⁸ What's in a name? As the Central Administration of Oxford University first pointed out 'materials science' is incorrect English. It should be 'science of materials'. Similarly, 'materials science and engineering' is ungrammatical. It should be 'science and engineering of materials'. Occasionally one sees 'material science'. That is correct English because 'material' can be used as an adjective, but it does not mean the same as the 'science of a material' - it means the opposite of 'immaterial science'! To avoid incorrect English and for brevity some university departments are called 'Department of Materials', which unfortunately is sometimes misunderstood as 'Department of Textiles'.

understanding of materials can provide much needed insight and sometimes predictions about the performance of materials in service.

A study⁹ in 2016 of the economic impact of TSM found that 80% of companies surveyed reported innovation as a result of TSM, 60% reported cost savings, 35% reported job creation and 30% reported revenue increase, with an average reported return on investment of almost a factor of 8. Simulation currently accounts for 5% of all publications added to the Science Citation Index and the number of TSM papers is growing at a rate of 5% per year - about double the average for all science.

1.3 Influences on my thinking about the PhD

The vision I outlined in the proposal in 2008 for the TSM-CDT brought together two strong influences on my thinking. The first was my own PhD experience with my advisor¹⁰ Professor Vasek Vitek at the Department of Materials Science and Engineering at Penn.

1.3.1 My PhD at the University of Pennsylvania

I had started a doctorate at Oxford University in 1977 with Vasek. He was then working at the Central Electricity Research Laboratories in Leatherhead, Surrey. He was offered a full professorship at Penn and, given the paucity of opportunities in UK universities at that time, he joined the 1970s brain drain and emigrated to Philadelphia. I followed him shortly afterwards to start a fresh PhD in September 1978 on a University Graduate Scholarship. My research involved a great deal of writing and running computer programs. Fortunately Vasek felt there should be more to a PhD in materials science than sitting in front of a computer terminal all day. He recommended I take some of the

⁹ G Goldbeck and C Court, *Economic Impact of Materials Modelling* (2016). <https://zenodo.org/record/44780>

¹⁰ PhD advisor is the American term for the PhD supervisor.

advanced graduate courses available in the Departments of Materials Science, Chemistry, Physics and Mechanical Engineering. I took his advice.

He also recommended I read some papers by J D Eshelby. Eshelby's papers remain the most elegant and inspiring I have studied in theoretical materials science. When I left Penn in 1981, having completed my PhD in a little over two years, I returned to Oxford with a deeper and broader knowledge of materials science, physics and mathematics.

1.3.2 The PhD at Oxford University

Following eight creative and productive years on a Royal Society University Research Fellowship I joined the faculty at Oxford in 1991. I noticed that many of our PhD graduates¹¹ with first degrees in other disciplines knew less about materials science than our first year undergraduates. Their acquaintance with materials science was limited to their very narrowly defined research topic. They 'knew everything about nothing' in materials science and yet they were getting a doctorate from Oxford in the subject. These students were receiving the traditional PhD experience described earlier. My observations were dismissed by my faculty colleagues on the grounds that in the three-year British PhD there was no time and no appetite for coursework. They held this view even though in subjects like Theoretical Physics at Oxford there was a suite of courses taken by first year PhD students and their PhD funding was also for three years. This became a source of constant frustration for me. I could not recruit our own undergraduates for a PhD because they were so weak in physics, mathematics and computing, while physics graduates knew virtually nothing about materials science. Nearly two decades later I discovered

¹¹ The PhD degree at Oxford is called the DPhil, but to avoid confusion I use PhD for the Oxford degree as well.

many others around the World were experiencing exactly the same dilemma.

1.3.3 David Pettifor's Materials Modelling Laboratory

The second influence on my thinking about a PhD was Professor David Pettifor. David came to Oxford in 1992 to take up the Isaac Wolfson Professorship of Metallurgy. He knew what he wanted to achieve at Oxford. Although he was a theoretical physicist who worked on fundamental aspects of materials he understood that materials science is a multi-disciplinary subject involving physicists, chemists, materials scientists and engineers. Today one would add biologists, mathematicians and computer scientists.

David observed that when these people modelled a material they would consider it from quite different points of view. Chemists and physicists calculated its *electronic structure*, providing models and understanding of the bonding between the constituent atoms. Using this knowledge they would make predictions for example about its optical or magnetic properties.

Having a relatively simple model of how atoms interact in a material enables calculations to be made involving up to a billion atoms. Such *atomistic calculations* are undertaken by materials scientists to model the atomic structures of mobile defects in a crystal such as an advancing crack.

There are some materials in common use that consist of a single thermodynamic phase. But it is more common that materials contain two or more phases and this gives rise to microstructure - the sizes and shapes of the different phases and how they are arranged within the material. Even crystalline samples of single phases may display microstructure because they normally consist of agglomerates of many crystals forming 'polycrystals', such as polycrystalline silicon used in solar cells. The crystals are rotated with respect to each other and when

two such crystals meet there is a boundary between them. The network of these boundaries is a form of microstructure. There are other forms of microstructure related to the defects that can occur inside the material. The study of microstructure in all its forms, its alteration through heating and/or deforming the material and the relationship between the properties of a material and its microstructure, are traditional heartlands of materials scientists.

Engineers are more concerned with properties of a material at the level of a component, such as an aircraft wing or a hip prosthesis. The engineer understands that bonding between atoms in the material and its microstructure affect its properties. But to model a component as large as an aircraft wing it is not possible to include so much detail. Instead the engineer uses *constitutive relations* that treat the material, with all its internal structural detail, as a homogeneous solid. In principle these constitutive relations can be calculated by materials scientists. But in practice they are usually determined empirically through experimental tests on sufficiently large samples of the material of which they are representative.

As we pass from the electronic structure of a material, to atomistic calculations and then to its microstructure and finally to its constitutive relations we are looking at the material at increasing length scales, equivalent to using decreasing levels of spatial resolution in a microscope.

The properties of the material at each length scale are dependent on the properties at each of the smaller length scales. To capture these dependencies information has to be passed from one length scale up to the next in the length-scale hierarchy. David recognised that this requires communication between the different groups of scientists and engineers working at each length scale. This is partly a linguistic problem because each discipline has its own concepts and terminology. It also requires the development of new theory and models to *bridge*

the length-scales. He recognised that the way to achieve this goal is to bring chemists, physicists, materials scientists and engineers together to understand one another and to build bridges between the length scales. This was his vision for the *Materials Modelling Laboratory* (MML) at Oxford. It was the first of its kind when it was opened on May 23, 1997. He also set up seminars for everyone involved in the MML so that people from one discipline could learn how materials are studied by people in other disciplines. The seminars were key to enhancing communication between the discipline silos.

David did not share my enthusiasm for coursework for our PhD students. He had no need for it because his research was in mainstream physics and he attracted excellent physicists to work with him. But since much of my research was in mainstream materials science I struggled with the dilemma I described above.

1.3.4 (Materials Modelling or Computational Materials Science?)

David Pettifor was sometimes asked why he called his centre a *Materials Modelling Laboratory*, rather than a *Computational Materials Science Centre*, which is now more widely used in the US and UK. His reply¹² was characteristically forthright:

Solving numerically quantum mechanical or classical equations is not the key step in providing insight into the complex world of materials and their properties. The critical step, the creative step, is finding a model that encompasses the dominant mechanisms of the complex process one is wishing to describe.

¹² Interview of Professor David G. Pettifor by Bernadette Bensaude-Vincent. <https://tinyurl.com/rb3382o>

If the objective is to *understand* better some property or process in a material a model has to be developed first. A computation framed by the model enables the model to be tested against real experiments. There is a relative abundance of people capable of developing computational methods and writing computer software. But there are far fewer who have sufficient insight and understanding of materials to create successful models. I believe this is why there has been a recent surge of interest in machine learning and artificial intelligence in materials science. Machine learning replaces the quest for *understanding* with *fitting, interpolating and extrapolating data* from experiments or computations. It also places bounds on the accuracy of the extrapolations. But it is difficult to see, for example, how data alone will enable the identification of *mechanisms* of processes in materials. For that one needs an understanding of the physics of defects in materials to develop plausible mechanistic models and how the mechanisms are likely to vary with the operating conditions in service.

1.4 Bringing it all together at Imperial College

It was only when I moved to Imperial College that I was able to action the two major influences on my thinking of (a) coursework for PhD students as I had at Penn and (b) a multidisciplinary environment for PhD students like the MML at Oxford. In the next chapter I describe how creating the multidisciplinary environment started to happen soon after my arrival at Imperial College in January 2005 and resulted in the *Thomas Young Centre*¹³.

So far I have set out only the academic reasons for a radical new approach to the PhD in TSM. Once I started to work on the proposal for the TSM-CDT in 2008 I realised there was much more that should be done to improve the experience of our PhD students. Julian Walsh helped me to think ‘outside the box’ to develop the ethos we wanted to

¹³ <https://www.thomasyoungcentre.org>

create. This included the mentoring of students, the extra-curricular activities we should provide, how to empower students and how to enable them to give serious thought to their future careers.

Julian was an alumnus of the College who returned after a successful career with BP to put his passion and experience at the service of his *alma mater*. This book will describe how we put the personal and academic development of our students at the centre of all our activities in our CDT.

My experience as a PhD student in the US had led me to the same thinking that had resulted in the introduction of the ‘New Route PhD’ in the UK. This is hardly surprising since the New Route PhD was based on the North American PhD. Recognising also the need for imaginative training in professional skills after the Roberts report and the need for a multidisciplinary environment for a PhD in TSM, I was well placed to write the proposal for our CDT in 2008.

2. The Thomas Young Centre

On January 1, 2005 I began my new job as Professor of Nanotechnology in the Condensed Matter Theory Group of the Department of Physics at Imperial College. A month later I was contacted by Professor Marshall Stoneham from the Department of Physics and Astronomy at University College London (UCL). We knew one another well, having co-supervised some doctorate students when Marshall was at Harwell and I was at Oxford. Marshall wanted my help to spread a rumour he had shamelessly started about setting up a centre in London for ‘materials modelling / simulation / theory’. He was thinking of something like the Institute for Theoretical Physics at Santa Barbara with visiting senior scientists, focused discussion meetings and seminars. His idea was enthusiastically received by colleagues at UCL and he wanted to get Imperial College involved too.

I was immediately attracted to his idea. It was a mechanism to bring together the excellent scientists and engineers working across London on materials. It would also provide the multidisciplinary environment I believed was essential for PhD students in TSM. Professor Mike Finnis from Queen’s University Belfast became the founding director of the centre in January 2006 when he was appointed to a Professorship in Materials Theory and Simulation¹⁴ held jointly in the Department of Materials and the Department of Physics at Imperial College. The centre involves University College London, King’s College London, Queen Mary University of London and Imperial College London. The first task was to find a name for the centre with which everyone could agree. Mike found Andrew Robinson’s fascinating biography¹⁵ on Thomas Young. Since Thomas Young did seminal work on materials,

¹⁴ more bad English!

¹⁵ *Thomas Young. The last man who knew everything*. Oneworld Publications: Oxford (2006). ISBN 9781851684946.

among very many other things, and he had lived in London, his was an ideal name to attach to the centre. The Thomas Young Centre, or TYC, was born, with the strapline ‘The London Centre for Theory and Simulation of Materials’.

It was quickly realised that each institution had to find space to accommodate TYC activities and a contribution to the running costs of the centre. Neither was straightforward as there was no mechanism to apply for funding from the usual external sources to support a multi-institutional centre like the TYC. But eventually, after several false dawns, each institution found a way to fund TYC activities. At Imperial it was achieved by each participating department paying a fixed annual contribution. Space was also found eventually at Imperial to accommodate some students and post-docs associated with the TYC. But like the academic staff, many remained scattered across the College in nine participating departments. On November 10th, 2006 the centre was formally opened with a lecture held at Imperial by Professor Michele Parrinello. The TYC web-site was established and a steady stream of senior scientists from all over the World started to visit London to give lectures and courses.

The TYC has become a focal point for industry to tap into the expertise among more than 100 academics involved in it. Perhaps most significantly PhD students and post-docs in the four participating London colleges can meet and interact with each other and with visiting senior scientists.

The TYC is a bottom-up initiative, conceived by academics who worked together across four institutions to make it happen, drawing on support from those institutions. There is no longer a single director. Instead there are co-directors in each institution who form the Senior Management Team and who report to their respective institutions on TYC matters. One of their primary roles is to ensure the TYC remains relevant and useful to the membership. The TYC executive committee,

consisting of the senior management team and other academics from the four institutions, considers proposals for international symposia, conferences and workshops and for visiting scientists. There are lunchtime seminars given by students in each institution and highlight seminars and evening soirées given by senior scientists to the whole TYC. There are also focused meetings organised for industry where academics in the TYC speak about research on a subject of particular industrial interest.

Marshall Stoneham's vision has been realised. The TYC has made London well known nationally and internationally for excellence in TSM. It provided the perfect research environment for the proposal I wrote in 2008 for our CDT at Imperial.

3. The professional development of PhD students

3.1 Background

The CDTs pioneered by EPSRC brought together the professional skills advocated by the Roberts report and the 4-year New Route PhDs. CDTs reduce the risk of lone PhD students struggling by themselves with their research by introducing cohorts of 10-20 students. In a cohort-based approach students help each other with coursework in the first year, they organise brain-storming sessions to help each other with their research and they run journal clubs and social events. In some CDTs students are empowered by being able to choose their research topic *after* they have become acquainted with the subject. They may also get involved in outreach and public engagement activities and they may invite leading academics and industrialists to CDT conferences. Up to 25% of the PhD can be allocated to taught interdisciplinary coursework at Masters level. That dealt with the problem of former 3-year and 3.5-year UK PhDs ‘knowing everything about nothing’ in TSM. In CDTs students are immersed in a research environment that enables them to *broaden* their horizons in research and training.

This chapter sets out how we built upon some of these ideas through our cohort mentor scheme and our suite of professional skills courses.

The multi-disciplinary theme of the TSM-CDT is ideally suited to a cohort-based approach. Irrespective of their disciplinary background students undertake the MSc in TSM in year 1, exposing them to theoretical concepts and computational tools required for understanding and simulating materials. Regular problem-solving tasks facilitate peer-learning through collaborative work. Our group-based projects (see chapter 4) have enthusiastic support and involvement from industry and would be much more difficult to deliver with a group

of students working independently in traditional PhDs. In his 2015 report, the External Examiner of the MSc, Prof Graeme Ackland (University of Edinburgh), noted that:

The course structure encourages working together and it was clear that the students were driving up each others' standards by doing this. There is a strong sense of belonging to the cohort which is actively fostered by the course team in a number of ways.

3.2 Cohort Mentors

Cohort-building is central to the ethos of our CDT and is led by a dedicated cohort mentor for each cohort. Cohort mentors are academic members of staff, drawn from the participating academic departments. The role of the cohort mentor is to provide welfare and pastoral care and to help set the ethos of our CDT. They are also lightning conductors for any problems with the coursework in the first year and any problems with the PhD research supervision in later years. In the cohort's first year the cohort mentor takes the cohort to lunch on Thursdays through term time. Any problems with teaching of the coursework are relayed by the cohort mentor at the Friday lunchtime meeting of the TSM-CDT Operations Board¹⁶. Such problems are normally resolved by Monday after the weekend. Students talk privately to their cohort mentor about any personal matters that are affecting them. If students have serious personal problems they are referred to the appropriate College services.

Once the research projects are underway it may happen that a student discovers they are unable to get on with a supervisor. The cohort mentor would then have a conversation with the supervisor to try to

¹⁶ The Operations Board deals with the day-to-day management of our CDT. It is chaired by the CDT Director and it has student representatives and the cohort mentors from each cohort and administrative staff. Students leave the meetings when confidential matters are discussed under reserved business.

resolve the matter. That is usually sufficient. But on a few occasions it has been necessary to find an alternative project and supervision, in consultation with the student. The CDT director has the authority to do this because the CDT owns the studentships. The cohort mentor sees the cohort as a whole once or twice a month during the PhD research, sometimes at specially organised social events.

The cohort mentors' time was fully costed in the proposal to EPSRC. The cohort mentor scheme was adopted by other CDTs at Imperial. It has also served as the template for the College's cohort mentoring policy for non-CDT based PhDs.

3.3 Professional skills

It is quite common in the UK to find that PhD students, and often their supervisors too, regard courses on professional skills as a waste of time, sometimes with good reason. EPSRC was looking for an injection of innovative thinking into these courses. We have put a great deal of thought into our professional skills courses, involving experts in their design and delivery. These courses have been shared with other CDTs within and beyond Imperial. Paying close attention to student appraisals the courses have improved year on year.

The combination of the suite of bespoke professional skills courses, the networking activities with other CDTs and the ample opportunities for student leadership, creates students who are rounded, confident and able to deploy their talents more effectively. As noted by our IAB:

The Board felt that the CDT students had a broader skill set for their careers than a standard PhD student. They felt that excellence in science and technology was almost a given with the calibre of students it attracts and that the real benefit of the CDT was that it adds value by educating and training visionary scientists and engineers capable of making transformative impact.

3.4 Research ethics

There is a mandatory one-day introductory course on research ethics in the first term of the MSc year on research ethics. The course is given by Marianne Talbot¹⁷, Director of Studies in Philosophy at the University of Oxford. Marianne defines research ethics as follows:

Research ethics is the discipline that studies the moral acceptability of the actions we perform when we conduct research and the ways in which we perform them.

The course covers plagiarism, scientific misconduct, whistle-blowing, open access publishing and it looks at case studies.

In subsequent years there are one-day courses that consider the ethics of particular research areas germane to TSM.

3.5 Authenticity

This is a mandatory course developed by Piero Vitelli¹⁸ taken by students soon after they have completed the MSc. The course is about working in teams to create effective presentations on a particular theme in a limited time. In the process students learn about giving and receiving feedback, self-awareness and personal impact.

David Trevelyan, a student who attended the course, wrote the following comment about it:

The real benefit of the course was not, as some might have expected, in learning how to work in a team environment. Instead, the students were treated to a uniquely open atmosphere in which they were offered sometimes startlingly pertinent feedback on their demeanour,

¹⁷ <https://mariannetalbot.co.uk>

¹⁸ <http://www.island41.com/>

personality, behaviour and their influence on those around them. Authenticity taught not what kind of behaviour to adopt, but instead how to recognise and understand it in oneself and others.

3.6 Career planning

This is a mandatory two-day course taken about half-way through the second year of the PhD research. The timing of the course gives students time to strengthen their CVs by undertaking an internship or another substantial extracurricular activity, while leaving the final year free to concentrate on the PhD thesis. It is taken with students from other CDTs forming a group of about 40 students. I have worked with expert careers advisors Dr Helen Goulding¹⁹ and Jane Pooler from the Imperial College Careers Service to develop the course, which we have named “PhD - What Next?”. The course is given by five tutors experienced in mentoring students and people in industry.

A principal goal of the course is to make students aware that the number of academic positions available in science subjects is much less than the number of post-docs chasing them. Many of these students are unaware of fulfilling careers outside academia. According to data²⁰ published in 2012 by the Institute of Physics, the average proportion of post-docs in physics in the UK each year who are appointed to a permanent academic post in the UK is less than 2%.

At the course students meet six professionals who finished their PhDs in physical science subjects a few years earlier and who have embarked on exciting careers. In a plenary session the professionals speak briefly about their career choices, how they got started and the career trajectories they envisage. This is followed by meetings between small groups of students and each of the professionals, where students ask detailed questions they have prepared. The professionals come

¹⁹ <http://www.quercustraining.com/about.php>

²⁰ <https://tinyurl.com/qqs42wo>

from a diverse range of sectors including manufacturing industry, science policy, science journalism, banking, startups, teaching, charities, construction and more. Only one of the professionals is an academic. For those who wish to pursue an academic career there is an hour-long discussion with a senior academic about what the job entails (it is not what most students think it entails) and the different routes to becoming an academic member of staff. Those not interested in an academic career can choose between an hour long introduction to assessment centres, or a general question and answer session about careers.

Before the course each student identifies an advertised job they find attractive and writes a letter of application and their CV. Before the course the letter and CV are reviewed by tutors in relation to the job advertisement. At the course the student receives one-to-one feedback about their letter and CV. They also receive feedback from tutors about their performance in practice interviews at the course.

This course has received exceptionally high praise from students, with some describing it as life-changing.

University departments of non-vocational subjects like physics often deny the need for them to expose students to careers outside the cloisters of academia²¹. It is clearly not enough to rely on university careers services, no matter how excellent they are, to tell students about the exciting and fulfilling career paths available to them outside academia, because far too many students in non-vocational subjects want to become academics.

In September 2015 Vitae²² published the results of a survey of the career aspirations of 32,280 research staff in the sciences, arts and

²¹ <https://tinyurl.com/usksncy>

²² Vitae is a non-profit programme, part of the Careers Research & Advisory Centre Ltd, with the aim of enhancing the professional development of researchers.

humanities in 72 higher education institutions in the UK²³. Research staff were defined as individuals whose responsibility is to conduct research and who are employed for this purpose. It excluded technicians and others in roles supporting research and it also excluded those in established academic posts such as lecturers and professors. There were 8,962 respondents, of which 77% anticipated an academic career, with 43% aspiring to work in a research and teaching role and 34% in a pure research role within higher education. 60% expected to achieve an academic career. These were very similar proportions to those reported by Vitae in 2013. These numbers are far too high and they indicate a total failure of higher education institutions to open the eyes of students to fulfilling career paths outside academia.

For researchers aspiring to become academics, having to leave the academic world because they are unable to secure an academic position is viewed as a personal ‘failure’. It is surprising that successive UK Government Ministers for Universities have not asked universities what they are doing about this problem. It is a problem because the overwhelming majority of PhD students pursuing academic careers are ultimately frustrated and disappointed. It is also perverse because these university departments are not funded to maintain a pool of highly skilled PhD graduates to compete for the small number of academic positions when they become available. They are funded to educate and train these students for the benefit of the wider community.

²³ <https://tinyurl.com/rwrv9yf>

3.7 Science communication

This three-day course was pioneered by the CDT on Chemical Biology²⁴ at Imperial College. In our CDT it is taken in the second year of the PhD research. It is led by Gareth Mitchell²⁵, with support from Dr Robert Sternberg²⁶ and Dr Claire Ainsworth²⁷. Gareth lectures in broadcast and written journalism for the renowned MSc course on Science Communication at Imperial College and he also presents the weekly technology programme *Digital Planet* on the BBC World Service. Robert designed the MSc in Science Media Production at Imperial College, which focuses on film, television and radio broadcasting. Claire is a freelance science journalist. Students are introduced to the elements of good storytelling and the presentation of news features about science on television and radio. They get hands-on experience of recording and editing their own short features and they record a twenty-minute show ‘as if live’ in BBC Broadcasting House in London.

3.8 Outreach and public engagement

CDT students are offered professional training in outreach activities for a wide variety of audiences by Dr Simon Foster. Simon is the Outreach Officer for three CDTs at Imperial College. Chapter 6 describes some award-winning examples of student outreach and public engagement activities.

²⁴ <https://www.imperial.ac.uk/chemical-biology/cdt/>

²⁵ <https://www.imperial.ac.uk/people/g.mitchell>

²⁶ <https://www.imperial.ac.uk/people/r.sternberg>

²⁷ <http://claireainsworth.com/>

3.9 Masterclasses

Masterclasses are organised twice a year where students in all four cohorts of the TSM-CDT can chat with a distinguished and inspirational person in an informal setting. Speakers have included Sir William Atkinson - Executive Headteacher of Phoenix High School in Shepherd's Bush, Sir William Wakeham - former Vice Chancellor of Southampton University, Dr Vivienne Cox - former Executive Vice President and Chief Executive of BP's gas power and renewable business, Professor Paul O'Brien - Head of the School of Chemistry at the University of Manchester and founder of Nanoco Technologies Ltd and Professor Dave Rugg - Senior Fellow in Materials at Rolls-Royce.

Other masterclasses are organised in the Hermes summer schools, as described in chapter 6.

3.10 Visiting senior scientists

The following senior scientists spent a month in our CDT interacting with students and giving short courses:

- Dr Jerry Tersoff, Principal Research Staff Member, Thomas J. Watson Research Center, Yorktown Heights, NY USA.
- Professor Richard M Martin, Department of Physics, University of Illinois at Urbana - Champaign, USA.
- Professor Vasek Vitek, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, USA.
- Professor Dr Karsten Reuter, Department of Chemistry, Technical University of Munich.

4. The TSM-CDT

4.1 (The need)

In Chapter 1 I described how I came to the conclusion, prior to the introduction of any CDTs, that the PhD education and training in TSM in the UK was not fit for purpose. This is how I summarised the need for our CDT in the proposal to EPSRC in 2008:

The need for this CDT cannot be overstated: there are no longer any PhD graduates produced anywhere in the UK with a broad foundation knowledge of theoretical and computational materials physics. Undergraduates of materials science learn about the phenomenology of an ever-increasing range of materials but their mathematical training is almost always too weak to enable them to do more than apply standard simulation packages in TSM. But, as noted on p.8 of the Foresight Report on materials modelling in the UK²⁸, a particularly difficult but vital aspect of TSM is ‘knowing the science such that the limitations of the models [are] understood and the value of the answer assessed’. That is incompatible with treating simulation packages as black boxes.

On the other hand, undergraduates of physics (not students of materials) are exposed to virtually no materials physics, as opposed to solid-state physics. Students with good degrees in physics have been attracted to take PhDs in TSM, but because they have been taught so little about materials and because the focus of the PhD degree has been on research, they still know extremely little about materials physics when they graduate with a PhD. Over the past 20 years this has created PhD graduates in TSM who are unaware of some of the most fundamental aspects of materials physics, such as the concepts of

²⁸ <https://tinyurl.com/vuumaxj>

microstructure and its control through processing and the crucial roles of defects in materials.

Professor David Bacon of the University of Liverpool endorsed my assessment of the need in the UK for the TSM-CDT:

The description of the current situation in the UK is excellently summarised in the case you have made. It has been clear for some time that education in theory of materials that undergraduate students experience in physics and materials science degree programmes has declined to the point of almost non-existence. I think this situation has arisen from a combination of the level of theory current materials students can cope with and the pressure to cover a wider range of topics at the expense of depth in a few. It is not due to a lack of need for graduates who have some mastery of the theory of materials.

... I have found the search for suitable UK students for funded PhD projects involving TSM to be rather dispiriting in recent years. I suspect that most of my academic colleagues share that experience.

In further letters of support distinguished scientists in universities and national laboratories in the USA, France, Germany, Spain, Switzerland and Japan all recognised the same inadequacies in their own education systems. My assessment of the parlous state of education and training in TSM in the UK had resonated around the World. The following is a selection of quotations from their letters.

Professor Ladislav Kubin, ONERA, Paris wrote:

... it is less and less common to find PhDs, graduate engineers, sometimes young researchers, having a sufficient background to at

least identify at which scales and by which means a given problem has to be treated. Young theorists have no idea about the realities of materials science, whereas mechanical engineers are too often not able to go beyond routine modelling. In the past years, for instance, I heard many colleagues complaining that it was becoming easier to obtain PhD or post-doctorate positions than to find even moderately decent candidates to fill them.

In his final sentence Professor Kubin echoes Professor Bacon's point that it is very difficult to find suitable applicants for funded PhD projects, or post-doctoral positions, in TSM. It is often easier to get the funding for these positions than it is to find suitable people to fill them.

Professor Sidney Yip at MIT wrote:

I believe the proposed Centre will have exceptional worldwide impact... As a member of the multiscale materials modeling community since the early days, I have indeed observed the problem that you propose to address, the decline of undergraduates strong in theoretical and mathematical skills, as well as understanding of materials science. This is a matter of global concern, ...

Dr Alfredo Caro at Lawrence Livermore National Laboratory, USA wrote:

I firmly believe that the idea is based on a correct diagnosis of the present situation not only in the UK, as Prof. Sutton says, but in many other countries as well. Materials science has evolved dramatically in the last decades and the traditional barrier separating metallurgy from physics does not exist anymore. However, the curricula of most universities still do not reflect the strong need of basic mathematical

and theoretical tools needed to perform actively in the field of modern materials science.

4.2 (Mission)

Having identified the need for our CDT, its mission became the following:

To create a new generation of scientists and engineers with the theoretical and computational abilities to model properties and processes within materials across a range of length and time scales.

This has remained the mission because the need continues. In 2012 we established a strong collaboration with the aerospace and nuclear businesses of Rolls-Royce in Derby (see chapter 6). In the proposal we wrote in 2013 for a further five years of funding we made rebuilding metal physics one of our central goals. The physics of defects in metals was a great strength of UK physics in the fifties and sixties, but research funding for it declined during the nineties even though it remained highly relevant to companies like Rolls-Royce. Since 2012 the research of our TSM-CDT students on defects in metals and the evolution of metallic microstructures under irradiation has been world-leading (see chapter 6).

4.3 (Strategy)

The first strand of our strategy was to recruit mathematically able scientists and engineers, with a strong inclination for theory and computation, and provide them with a rigorous education in TSM leading to an MSc degree.

The second strand was to involve initially 20 academics across 4 departments in the Faculties of Natural Sciences and Engineering at Imperial to deliver the teaching and supervise research projects. These

numbers eventually grew to more than 80 academics from 9 departments at Imperial departments and 17 partner academic and industrial organisations.

The third strand was to bring our CDT students into the unique research environment of the TYC and to involve academics in the TYC outside Imperial in the development and supervision of research projects for our CDT students.

The fourth strand was to work closely with our industrial partners, to translate their complex problems into viable PhD research projects and to involve them in teaching in our CDT as well as research.

The final strand was to work with experts to create bespoke, imaginative and worthwhile professional skills courses to prepare our students for their future careers.

To recruit students with the required mathematical ability we targeted students in physics and engineering who would otherwise choose PhDs in theoretical physics and engineering subjects. We have also recruited a smaller number of students with first degrees in materials science and chemistry. With rampant grade inflation in UK universities²⁹ we have always sought students with first class honours degrees and more than 80% have firsts or overseas equivalents with the remainder obtaining a high upper second class honours degree. We have used some of our significant industrial funding to support non-UK EU students and a few students from outside the EU. The non-UK EU students have consistently raised the level of educational attainment of the intake. This is probably because the pool of EU students is much larger than the UK pool and those that seek a UK post-graduate education are usually self-selecting in the upper tail of the distribution of academic ability.

The recruitment of outstanding students by our CDT attracted a rapid increase in the number of academic staff involved in its teaching and

²⁹ <https://tinyurl.com/qks5r9r>

research. In the 2017 mid-term review we reported there were 71 project supervisors in 9 departments at Imperial and 16 external organisations (both academic and industry). A requirement of the supervision of each TSM-CDT research project is that there are *two* supervisors with complementary expertise at different length scales. Normally the two supervisors come from different departments and often they have not jointly supervised a student before. This is an example of the change of culture the TSM-CDT has brought about within Imperial College, raising the level of interdepartmental and cross-faculty collaboration.

4.4 Student recruitment

Formal applications and references are submitted via Imperial's online system. Shortlisted applicants are invited to interview with the TSM-CDT Admissions Tutor and at least one other member of academic staff. Applicants from remote locations are interviewed via video conference. A week beforehand applicants are sent three problems at the level of second year undergraduate and of such a nature that an applicant from any physical science or engineering background should be familiar with at least one. Applicants are asked to prepare a solution to one of the problems of their choice and to go through it at the interview. This provides a springboard for unseen questions that probe deeper understanding of how the mathematics reflects physical principles. We find this approach discriminates effectively between applicants with excellent academic records on paper. The College Graduate School identified this as an example of best practice and it has been adopted by other groups at Imperial. All applicants are given the opportunity to have informal discussions with students already in our CDT, who provide a student-led tour of the campus.

In the 2017 mid-term review we reported that although the majority of our students come from physics departments, over 40% come from

other disciplines, including materials science, chemistry and engineering.

4.5 (Coursework in the first year)

The content, structure and assessment of the coursework evolved with experience and the introduction of new thinking. A major restructuring took place at the time of the first application to renew funding for our CDT in 2013. This restructuring increased industrial engagement and enhanced the development of students' independence. It also provided more opportunities for peer-learning, particularly group projects. It expanded computational training and it involved a wider range of academics and created more time for the MSc research project. The structure and content of the coursework presented here is the result of all these changes and innovations.

During the first term students take six core modules:

- Thermodynamics of materials
- Transformations in materials
- Electronic structure of materials
- Elasticity and crystal defects³⁰
- Mathematics for the theory of materials
- Computational methods for materials.

Each of the first four courses consists of 20 hours of lectures and problem classes. The mathematics course has 24 lectures and 8 problem classes. The computational methods course consists of 20 hours of lectures and hands-on computational labs. With the exception of the computational methods course, all are assessed by problem sets and written examinations in January.

³⁰ This course is called *Classical field theory of materials* to make it more attractive to physicists.

During the second term students continue the core computational methods course with a further 20 classes, including group mini-projects. They also take two further core modules: (i) the Group Research Strategy Project and (ii) Methods of Simulating Materials. In addition, students choose two from four advanced options that build upon the material covered in each of the first four core courses of the first term. These advanced option courses promote independence through a combination of seminar style delivery and directed reading. They are assessed by regular coursework and an oral examination at the end of term 2. In term 3 and throughout the summer, students focus exclusively on a 4-month research project serving as a taster of their PhD project, for which they write a thesis assessed by two independent academics.

4.6 Group projects

We have developed two group projects for the MSc:

- Group Research Strategy Project
- Group Programming Project

They illustrate what can be accomplished with a cohort-based approach to PhD education and training, that would be much more difficult to organise in a traditional PhD programme.

The Group Research Strategy Project (GRSP) grew in part out of my experience, starting in 2012, of talking to engineers at Rolls-Royce in Derby about the issues they faced with a range of materials across their aerospace and nuclear businesses. It takes time to do the background research and think through how a complex engineering problem can be simplified, without sacrificing relevance, into a well defined, feasible research project that can be given to an able PhD student to work on for three years. Formulating a research strategy to address a complex industrial problem in a meaningful and useful way is a creative process of *translation*. The process normally involves the creation of a model

‘that encompasses the dominant mechanisms of the complex process one is wishing to describe’, to quote David Pettifor again. It is an essential skill that has to be honed by anyone who wants to model the complex materials problems faced by industry. However, it is not a skill that is recognised by those who have not themselves engaged in university-industry interactions. The point of the GRSP is to give our CDT students an opportunity to develop this skill by asking them to create a strategy for research on a specific industrial problem.

In the GRSP students work in groups of 5 to 8. They are introduced to a materials problem in industry by one of our industrial partners, who plays a key role in the project. Each group is tasked with producing an EPSRC research proposal to address the problem. They are encouraged to visit the company and to discuss the project further with the industrial partner. They are assessed on the quality of the proposal and on their performance at an interview, run like an EPSRC panel interview. The interview panel includes the industrial partner, the EPSRC contact for our CDT, the academic who has overseen the project and the TSM-CDT Director. Students have the whole of the second term to work on their proposal, alongside their other coursework. They brainstorm the problem, divide the research and writing tasks among themselves, think through the resources they need and their costings and arrange visits to the company. They are free to propose experimental, theoretical and computational research involving post-docs and/or students. They also have to decide how they are going to present their proposal at the interview.

There is no doubt students find the GRSP difficult. It is probably the first time they confront a problem for which there is no known solution. Some find it an unnerving experience, others relish the challenge. They are encouraged before they start by a discussion with Professor Dave Rugg, Senior Fellow in Materials at Rolls-Royce, who tells them about the intellectual challenges of industrial problems with examples of how

they were tackled. The analytic and team-working skills students develop through the GRSP will be useful to them in any career path they follow.

In the Group Programming Project (GPP) students work together to write a modular materials simulation code from scratch, e.g. a plane wave density functional theory program. Working in groups of 5 to 8, students write a full specification of the modular structure of the program before writing any code and divide up the task of writing the modules among themselves. Writing software in a team is quite different from writing it by oneself and students learn, for example, about the discipline of version control. Alongside their other coursework, students were given the whole of the second term in the MSc year to complete the task. Their results were compared with those from a standard program called CASTEP. In the first year GPP was run it was assessed by Prof. Mike Payne, original author of the commercial CASTEP code. He wrote:

The students did not have a background in professional software engineering and some had very limited experience of software. Against this background then the level of achievement in the GPP was outstanding - writing a fully modular plane wave pseudopotential code validated and tested against a standard reference code CASTEP. This experience will be invaluable to the students whatever their future level of involvement with software and the skill set gained, not least the team-working which was central to the entire GPP, will make the students extremely well placed for almost any future career.

Initially students were offered the choice of either the GRSP or the GPP. Perhaps not surprisingly they tended to prefer the GPP. However, we withdrew the GPP after our IAB said the GRSP was an experience too valuable for any of our CDT students to miss. The principles of the

GPP were incorporated into the course ‘Computational methods for materials’.

5. The research project

5.1 The MSc research project

In addition to the coursework of the MSc there is a research project running from April to September. In the first month students write a literature review of no more than 3,000 words. Their research project begins immediately after the deadline for the literature review. Each student gives a 10-minute presentation about their project as part of the MSc Conference at the end of August. They also submit a 5,000-word report on their research a week later, which is marked by two independent assessors drawn from a panel consisting of principal supervisors. The assessors also receive a report from the student's principal supervisor about the student's achievements and skills and any external factors affecting the research.

The research project carries 40% of the total marks available in the MSc. Normally TSM-CDT students continue the same research project for the PhD in years 2-4. However, after submitting their MSc research project reports for assessment students are asked whether they wish to continue with the same project and supervisory team or to transfer to a different project. The supervisors are also asked to confirm their willingness to continue with the project. If they do not wish to continue then the TSM-CDT Director assists the student in finding another project. In this way the MSc research project is a taster for the PhD research project and the student has the option to terminate it at the end of the MSc if it doesn't suit them.

5.2 Eligibility to continue to the PhD research project

Provided a student has obtained an overall mark of at least 60% in the MSc they are eligible to proceed to the PhD in years 2-4 and to continue to receive the same level of funding from the TSM-CDT as

they received in year 1. If a student obtains an overall mark between 50% and 59% in the MSc, they pass the MSc and they may proceed to the PhD but any funding they received from the TSM-CDT is terminated. It is a rule at Imperial that students receiving an overall mark of less than 50% fail the MSc and they are ineligible to proceed to the PhD.

5.3 Student empowerment

A CDT owns the funding for the PhD studentships from EPSRC. In contrast to the traditional PhD, where the supervisor or the department owns the funding, the funding follows the student wherever they choose to undertake their research. Students are empowered by having the freedom to choose their PhD project from a wide range of proposed projects. They make their choice at the end of the second term when they have learnt about the subject. Supervisors, including those from industry, have to ‘sell’ their projects to students.

5.4 Creation and vetting of research projects

Research projects are solicited each autumn and proposals are submitted in early January using a standard form. Projects have at least two supervisors but in all cases no more than three, with a principal supervisor, who must be a member of Imperial College, with overall responsibility for monitoring and reporting progress. In addition, collaborators may be named, who are theorists or experimentalists, based in academia or industry. They contribute to the research by assisting the student from time to time. Supervisors and collaborators are identified on the application form, where their respective roles are differentiated clearly.

To ensure a fair distribution of studentships supervisors may be named normally on no more than two project proposals as principal or co-supervisor. Exceptions to this rule are subject to approval by the

Research Board, which comprises the heads of the participating departments, or their deputies, and the TSM-CDT Director. Supervisors are encouraged to diversify their collaborations by submitting proposals with another supervisor with whom they have not worked before.

The Research Board vets the project proposals to ensure they meet the five criteria listed below. On the advice of the IAB, the Research Board ranks the proposals and a shortlist of no more than 3 projects per student, up to a maximum of 30 projects, are passed to the students to avoid overwhelming them with choice.

Project proposals are not automatically carried over from previous years. Projects that were not successful in attracting students in previous years may be resubmitted.

Projects selected by the Research Board are presented to students in February. Supervisors of approved projects are invited to make a short presentation about their projects to the cohort. Students are encouraged to have further discussions in private with supervisors about projects that interest them. Over a period of about two months students make a ranked selection of three projects. The Director then tries to satisfy students' preferences in consultation with potential supervisors. With the help of the Director students are also free to propose their own projects provided they satisfy the selection criteria listed below and have made suitable supervision arrangements.

5.5 (Selection criteria for research projects)

It is essential that the process to approve research projects by the Research Board is transparent. The following five selection criteria are published by the TSM-CDT:

- The project must be about theoretical and/or computational aspects of materials of some current or anticipated use to society. While we encourage proposed projects to be closely related to experimental work a student will not be asked to carry out any experimental work him/herself.
- The project must be interdisciplinary. Normally this requires that it is explicitly multi-scale, spanning more than one length or time scale or both. For projects involving the development of software for global use the interdisciplinarity must also be explicit, for example by involving experts in numerical algorithms or computer science.
- Projects will normally have two supervisors from independent research groups. The principal supervisor is responsible for monitoring and reporting progress. In exceptional circumstances, to be specified on the application form, there may be a third supervisor. In all cases the principal supervisor must be a member of Imperial College, with expertise on theory and simulation of materials. Potential supervisors must meet the requirements of the College to supervise postgraduate research students. The expertise of the supervisors will reside at complementary length and/or time scales to enable the project to involve explicitly the transfer of information between different scales. For software development projects, the complementarity of the supervision team must also be clear. There may also be collaborators. Supervisors and collaborators are identified on the application form, where their respective roles are differentiated clearly. Supervisors and collaborators may be in industry, a government laboratory, or another higher education institution and they may be experimentalists.
- The scientific excellence of the project will be assessed against the risks, which should be explicitly identified on the

application form. No funding from the TSM-CDT is available for students who take more than three years after completing the MSc. A plan B should be identified on the application form in case the project fails to deliver any results after 18 months.

- All academic supervisors are expected to be willing to contribute to the delivery of the TSM-CDT if the proposal is approved, either through its teaching/training, or its management. Supervisors are asked to consult a check-list of TSM-CDT roles to indicate how they will contribute if they are not contributing already.

In 2013 when we applied to EPSRC for a further five years of funding we identified two priority areas of research: (a) the physics of metals and (b) the development of software for global use to simulate materials. In that round of applications a cognate CDT was established at Imperial on Advanced Characterisation of Materials (ACM). To work with this new CDT we developed the idea of ‘interface projects’ where a student from TSM and one from ACM collaborate on a combined theoretical and experimental approach to the same research topic. Finally, following a suggestion from our IAB, we introduced the idea of ‘cluster’ projects where two or more students work on different aspects of a larger project. The supervisory teams of cluster projects must not be the same. The idea of cluster projects was to make the research more ambitious by addressing larger problems, in a similar way to EPSRC programme grants. Proposals for projects on (a) the physics of metals, or (b) software for global use to simulate materials, or (c) interface projects with the CDT on ACM, or (d) cluster projects, were encouraged and given a higher priority in the selection process by the Research Board.

5.6 Monitoring progress of the research project

Imperial College has well defined processes for monitoring progress of PhD projects throughout their duration. Progress is assessed by an independent member of academic staff in addition to the principal supervisor, through written reports and interviews at which the student presents their work orally. Normally the same independent assessor is used throughout the student's PhD to provide continuity.

It is expected that the thesis is submitted within 48 months from the initial registration for the PhD. That corresponds to the end of year 5 in the TSM-CDT because students are registered for the PhD only at the end of the MSc-year. However, as stated before, TSM-CDT funding ends after 48 months. Any periods of absence formally registered with the College, for example due to illness or undertaking an internship with a company, are taken into account in the calculation of the 48 months.

In addition to the above formal processes to monitor progress, students in our CDT see their cohort mentor regularly throughout the PhD. These meetings are private when necessary. There have been occasions when these meetings have proved crucial to the eventual success of the PhD by enabling students to raise their concerns, such as their supervision and personal problems. Students also give a lunchtime seminar in the TYC in year 3 and they present their research at the TSM-CDT Conference in the summer of year 4. Members of the IAB are invited to the TSM-CDT Conference, which is held a day before the IAB meeting.

6. The mid-term review of 2017

In 2011 EPSRC conducted a mid-term review of all its CDTs funded in 2009. Considering our CDT had been running for less than two years the feedback we received from EPSRC was encouraging:

- The strong links with other Imperial Physics CDTs, other universities and research centres is very positive.
- The theory focus of the centre is a strength and this approach to materials simulation appears to be creating new collaborations within the host institution.
- The centre must increase EPSRC student numbers to hit the 50 student target over the next three cohorts.
- The strong outreach programme, the centre's project development process and ethics teaching are all areas of best practice.

At the beginning of October 2016 all CDTs funded by EPSRC underwent another mid-term review. This review was much more thorough, requiring the completion of a very detailed questionnaire. CDT directors had been given advance notice of the review in July 2015 to enable them to plan the workload and start collecting the data.

Our completed questionnaire of thirty pages of single space text and tables was submitted on January 5, 2017. In addition, we submitted six case studies (CS), each of one page single space text, chosen to highlight some of the main achievements of our CDT. CS1 described our approach to interaction with industry, with particular emphasis on the relationship that we developed with Rolls-Royce; CS2 and CS3 described our activity in the two scientific focus areas that we had identified in the 2013 renewal proposal, namely software development

for global use and the physics of metals, respectively. The remaining three Case Studies looked in detail at our students' achievements in entrepreneurship (CS4), leadership of their peers in the discipline of TSM (CS5) and outreach (CS6).

In the first eight cohorts 94 students were recruited, of whom 26 had graduated. 24 were in employment, the remaining two having passed their PhD vivas only in November and December 2016. Of these 24: 11 continued in research related to TSM, among whom 2 had won prestigious independent fellowships; 5 had gone on to jobs directly relevant to TSM, among whom 3 were employed by industrial partners of the TSM-CDT; the majority of the rest were in employment, or had started their own companies, where they used the problem-solving, computational and software development skills they had developed during their time in our CDT.

Between October 2009 and December 2016 our CDT garnered over £3M of leverage to support studentships in addition to its EPSRC funding. £1.9M of this was associated with the three cohorts recruited since the renewal in 2013, in which 19 of the 37 students (on average six per cohort) we recruited were either fully or partly sponsored with funds external to the TSM-CDT.

At the time of the mid-term review the number of supervisors in the TSM-CDT had increased to 71 from Imperial and there were 16 external organisations (industry and universities) collaborating with the TSM-CDT. In the two cohorts who had most recently chosen their research projects 65% of those projects involved groupings of supervisors who had not co-supervised a student before. This demonstrates the change of culture the TSM-CDT had brought about within Imperial.

The second tranche of funding awarded by EPSRC in 2014 included 34 studentships and the unit cost of each was approximately £32k/year. In addition to student stipends this funding paid for the teaching of the

MSc course, the suite of bespoke professional skills courses, administrative support shared with another CDT and a contribution to the salary of the Outreach Officer shared with two other CDTs. It also included a travel budget to enable students to attend meetings with partners and attend conferences.

6.1 Case studies

Six case studies were submitted to EPSRC as part of the mid-term review of the TSM-CDT conducted in 2017. Some of these documents have been updated to include more recent information. There is some repetition in these case studies of material that appears elsewhere in this book.

6.1.1 CS1: Industry engagement, Rolls-Royce plc

The engagement with Rolls-Royce (RR) has been key to the TSM-CDT strategy to rebuild theoretical and computational metal physics in the UK, following decades of neglect. Its success is attributable to the effort that has been invested by both the CDT and RR to make the relationship work. It began in 2012 when Professor Adrian Sutton made ten one-day visits to the company to speak to senior engineers in Aerospace and Marine Divisions. These visits resulted in a report, co-authored by Professor Sutton and Professor Dave Rugg (Senior Fellow in Materials at RR), identifying research areas across the company where *physically based* modelling could have a significant impact. The report has contributed to a change of culture in the company and there is now a greater recognition that it is realistic to seek a mechanistic understanding of microscopic processes that limit service life of components. This complements the traditional approach of macroscopic continuum modelling based on empirically derived constitutive relationships.

In 2014 RR set up a *Global, Rolls-Royce plc, Physically Based Lifing Steering Group*³¹ to identify ‘key high level requirements in the area of physically based modelling and to generate plans and research to address them’. It meets twice a year in Derby with participants from RR-Indianapolis and academic RR-collaborators in the US phoning in. The creation of this Group was a direct result of the Sutton-Rugg report and Professor Sutton was invited to join it. The report also led directly to 3 RR-supported TSM-CDT projects jointly supervised by Professor Sutton in Physics and colleagues in Mechanical Engineering and Materials at Imperial.

Professor Rugg has directly contributed to the TSM-CDT delivery, through his membership of the IAB, his participation in the Authenticity residential professional skills training course and in the Career Planning Course. He has given a masterclass to TSM-CDT students and he has been the industrial advisor and assessor of a Group Research Strategy Project (GRSP) on cold dwell fatigue. Since GRSP has been made mandatory he explains to MSc students why it is so important to their training. Professors Rugg and Sutton organised an international workshop on cold dwell fatigue in Switzerland in 2014 with 30 participants from Europe and the US. They also brought about the first experiment on the X-ray free electron laser at Stanford California to involve an industrial participant. The analysis of the results of this experiment was led by Tom Swinburne, who was then a TSM-CDT student, and published in 2016.

Richard Broadbent in cohort 1 became an employee at RR in 2014. Although his PhD was on polymers he has made a major impact within RR, which is heavily based on metals and alloys. This illustrates the value of the MSc in providing a broad education in TSM. Despite the pressure on the headcount, the company invited another TSM-CDT student working on delayed hydride cracking to apply for a position

³¹ *Lifing* means the determination of the expected life of a component in service.

after his PhD, with a significantly enhanced starting salary reflecting his value to the company.

Professor Rugg writes:

The relationship between RR and the CDT is proving to be highly stimulating and valuable. The fundamental yet pragmatic approach to problem solving and a real appetite for complex industrial problems is a considerable strength of the CDT and it is of clear benefit to both our nuclear and aerospace sectors. The resulting students have inherent capability and learned skills that are highly attractive to Rolls-Royce, being suitable for technically challenging roles in the company with significant growth potential. I was a strong advocate for RR engagement with the CDT at the outset and had high expectations with respect to the depth of engagement, quality of people involved and tangible output. I have not been disappointed.

The time invested by the TSM-CDT in developing a long-term relationship with RR has not been exceptional. Similar efforts were made to establish successful collaborations with Culham Centre for Fusion Energy (CCFE) supporting 4 students, Baker-Hughes supporting 2 students, USAFRL / EOARD supporting 1 student, Argonne National Lab supporting 1 student, Element Six supporting 1 student, BP supporting 4 students, Materials Design supporting 1 student, NPL supporting 1 student and Toyota supporting 2 students. The additional TSM-CDT funding leveraged from these relationships amounts to ~£1.2M. In 2011 Imperial became a hub for the BP International Centre for Advanced Materials to work on Separations Membranes. The TSM-CDT played a key role in this successful bid as a result of the work by Richard Broadbent on polymer membranes.

6.1.2 CS2: Science quality and adventure: software development for global use

Software is established as a vital element of a modern research infrastructure³², enabling the computational modelling and simulation that forms the indispensable ‘third pillar’ of scientific inquiry³³. It is therefore central to the mission of the TSM-CDT as recognised by our close relationship with our project partner Materials Design Inc.³⁴ a materials modelling software company.

Computational methods are a core stream in the taught coursework of the TSM-CDT, spanning the first year of the programme. Following an introduction to the Linux operating system and coding in C++, students take a course in numerical methods that embeds best practice in software development by requiring the submission of assessed coursework via a version control system used by professional developers. The CDTs at Imperial share a Computational Methods Hub³⁵ that augments this provision with training in topics such as high performance computing.

An important evolution of the TSM-CDT in 2013 was the identification of two priority areas for research projects, one being software development for global use. This is a high risk area for PhD students. Typically, much work is needed before the developed software yields publishable outcomes and impact emerges over a long period of time. One very successful example involves a cluster of three projects centred on the ONETEP code for large-scale quantum-mechanical calculations of materials. This code is marketed by Dassault Systèmes BIOVIA to the commercial sector (over \$4M revenue to date) with a separate source distribution to academic groups.

³² <https://tinyurl.com/ta83keq>

³³ President’s IT Advisory Committee, Computational Science: Ensuring America’s Competitiveness (June 2005). <https://tinyurl.com/te7ynu6>

³⁴ <http://www.materialsdesign.com>

³⁵ <https://tinyurl.com/rfsmb9u>

Tim Zuehlsdorff created an efficient implementation of time-dependent density functional theory for electronic excitations, Niccolò Corsini coded a method for studying nanocrystals under pressure and Andrea Greco implemented flexible localisation of electronic orbitals and Brillouin zone sampling.

Industrial internships have grown in popularity as news of their benefits spreads through the cohort networks of the TSM-CDT³⁶. In the software sector these have included: (i) Tom Poole with Materials Design in Angel Fire, New Mexico (USA); (ii) Andrea Greco and Nicola Molinari with Bosch R&D in Boston (USA); (iii) Frederike Jaeger with Shazam Entertainment Ltd.; (iv) Vadim Nemytov with Materials Design in Paris; and (v) Jacek Golebiowski with BIOVIA in Cambridge. Dr Victor Milman, Senior Fellow at BIOVIA wrote:

Jacek's stay was something special. It is hard to believe how much he has achieved in a short period of time.

Several graduates of our CDT started careers as software engineers: Tom Poole with Materials Design; Fabian Renn-Giles with the digital music company ROLI; David Trevelyan with soundtrack generation company Jukedek; Tom Edwards with First Light Fusion; and Karlis Kramens with Cisco Systems.

The TSM-CDT has played a central role in preparing skilled graduates for their careers through the emphasis on software development in our programme that builds confidence, the introductions to industry through site-visits and the career planning

³⁶ Not all internships undertaken by our CDT students are on software or in industry. For example, Daniel Rathbone and Amanda Diez undertook internships in the Parliamentary Office of Science and Technology, where they learnt about science policy. Daniel worked with the House of Lords Science and Technology Committee. He is now Assistant Director of the Campaign for Science and Engineering.

course and by brokering internships. Dr Erich Wimmer, Chief Scientific Officer of Materials Design Inc. wrote:

The partnership between our company, provider of the high-end atomistic simulation platform MedeA, and the CDT has proven to be extremely valuable as it creates a bridge between leading academic research and industrial deployment of advanced simulation technology. In particular, trained software developers with expertise in cutting-edge methodology are in short supply. We have hosted two highly successful internships (Tom Poole and Vadim Nemytov) and hired the first after he graduated.

6.1.3 (CS3: Science quality and adventure: the physics of metals)

By 1975 theoretical and computational metal physics had virtually disappeared from UK physics departments. But the need for research into metal physics has increased steadily since the sixties as aerospace and nuclear power became more reliant on physically based modelling of defect-related mechanisms. For this reason the TSM-CDT identified the rebuilding of theoretical and computational metal physics as one of its priorities in 2013. It has led to some of the highest quality research in the TSM-CDT, attracting some of the most talented students to have entered TSM in decades.

Beñat Gurrutxaga-Lerma's PhD project was on modelling dislocation plasticity at very high strain rates caused by shock loading. Beñat discovered that existing methods of modelling dislocation dynamics violated causality when they were applied to shocks because they all ignore the finite time for elastic fields to propagate. To overcome this comprehensive failure he developed the theory and numerical algorithms to model dislocation dynamics using elastodynamics where the time dependence of the elastic fields is

treated explicitly. This was a world-first. The work led to more than 30 invited talks at international conferences. During his PhD Beñat published nine papers in prestigious journals, including one as sole author and an invited major review article. The Institute of Physics awarded him first prize for the best thesis in the whole of Computational Physics across the UK in 2014. Following his PhD Beñat won an EPSRC Doctoral Prize Fellowship followed by a Junior Research Fellowship at Trinity College Cambridge. He is now a lecturer in the School of Metallurgy and Materials at the University of Birmingham.

Tom Swinburne addressed the mobility of defects in metals in a highly original way. Using techniques from statistical physics he explained analytically the origin of the temperature-independent contribution to the lattice friction experienced by highly mobile defects. His analysis resolved a long-standing disconnect between molecular dynamics simulations and 60 years of theory. Tom identified the terms responsible for the temperature-independent mobility and evaluated them, finding perfect agreement with his own molecular dynamics simulations. As one referee of his Physical Review Letter noted:

This paper fills an important gap in computational physics, namely, the determination of the origin of the temperature-independent friction coefficient from fundamental lattice dynamics, by convincingly separating the localized nature of defect cores from canonical vibrations. The theoretical arguments put forward by the authors are potentially applicable to many other areas in defect dynamics.

Tom's thesis was published in 2015 in the prestigious Springer Theses series. He published four papers, one as sole author, during his PhD. After his PhD he was awarded an independent fellowship at

CCFE, following which he secured a highly competitive independent Eurofusion Researcher Grant. He is now a permanent member of research staff of the CNRS in Marseille.

Marc Coury derived the most general s, p and d orbital Hubbard-like Hamiltonians to describe strong electron correlations and presented them in ways suitable for practical calculations of defects in iron where magnetism resulting from these correlations is known to play a very important role.

Iacopo Rovelli developed a novel boundary integral method to model the evolution of cavities and dislocation loops in microstructures produced by irradiation. He used this formalism to model microstructural evolution of irradiated tungsten in fusion reactors.

Mitesh Patel's project with Rolls-Royce led to outstanding research on modelling the formation and dissolution of hydrides during thermal cycling in zirconium fuel cladding in pressurised water reactors. In contrast to existing approaches he deliberately avoided finite elements and derived analytic expressions for the stress fields of defects in anisotropic elasticity, enabling much faster and more insightful calculations.

Luca Cimbaro, also with Rolls-Royce, has calculated analytically the stress fields caused by oxide particles on grain boundaries ahead of cracks in Ni-based superalloys and used these fields to derive an engineering criterion for fracture.

With the exception of Beñat, who has a background in mechanical engineering, all these students have backgrounds in physics. They were attracted into metal physics by the intellectual challenges these projects presented and a desire to attack problems with technological relevance. None of these projects would have been conceived if the TSM-CDT had not existed, because there were no mechanisms to bring together physicists and engineers to create projects of such adventure. The excellence of the students our CDT has attracted and the

multidisciplinarity of the TSM-CDT environment have made these remarkable research achievements possible.

Professor Sergei Dudarev, Head of the Materials Modelling Group at CCFE, who was a co-supervisor for Tom, Marc and Iacopo, notes that:

[their contributions to] computational modelling of defects produced by irradiation in metals and alloys for advanced nuclear and fusion applications, is proving critical to the success of the program. Not only do they help to solve outstanding issues of major significance, but they also make a profound impact internationally, often representing CCFE at prestigious international conferences and delivering the message about the quality of research conducted in the UK on nuclear and fusion materials. Through their training at the CDT they acquire excellent team-working skills and this helps us expand links with academia in the UK and overseas.

6.1.4 CS4: Student entrepreneurship

Some of our students set up companies during their PhDs or soon thereafter, all of which are in the digital domain and rely heavily on computational methods and software development skills, central themes of TSM-CDT training.

Ben Kaube co-founded Newsflo Ltd in 2012, the first year of his PhD research. It was acquired by Elsevier in January 2015, where it ‘offers researchers and academic institutions a way to measure the wider impact of their work by tracking and analysing media coverage of their publications and findings’³⁷. Ben says:

The technical problem-solving skills fostered by the CDT left me perfectly equipped for the competitive world of software innovation.

³⁷ <https://tinyurl.com/th9gfae>

Newsflo grew out of the ICStartup + accelerator programme of Imperial Innovations and received seed capital from the Digital Science Catalyst Grant programme to develop the platform. Newsflo is used by some of the leading research institutions, tracking the contributions of tens of thousands of academics every day.

Ben also co-founded Kopernio³⁸ in 2016. Kopernio enables a user to access the full text of a scientific paper with one click by searching the internet for a version to which the user may have legal access through institutional or personal subscriptions. It also searches for full-text versions of the paper which do not require any subscription. It was acquired by Clarivate Analytics in April 2018. Ben is now the managing director of Kopernio. The Kopernio tool has been fully integrated into Web of Science.

Fabian Renn-Giles co-founded Fielding DSP³⁹, which provides an audio plug-in for harmonic distortion. The plug-in has been lauded by music industry experts. The following quote is from *Computer Music Magazine*, Jan 2013:

There are dozens of ‘make it louder’ plug-ins and compressors and saturators on the market. I find Fielding DSP’s approach unique. While generating harmonics which to our ears make signals appear larger and fuller, it does not suffer from the side effects of similar plug-ins, retaining a very clear, un-smashed signal.

³⁸ <https://kopernio.com>

³⁹ <https://www.fieldingdsp.com>

Fabian himself says:

I think the CDT was really unique in allowing students to pursue entrepreneurial ideas. The many master classes in the CDT, often from entrepreneurs, really highlighted this aspect.

Aeneas Wiener is Chief Technology Officer and co-founder of Cytora, a company that ‘generates real time data to help companies identify, manage and price risk’⁴⁰. Founded in 2014 Cytora uses advanced machine learning to turn billions of pieces of web-based information into structured, factual data describing where risk is distributed in the world. It is used by some of the largest insurance companies including AXA XL, QBE and STARR. Cytora has grown with offices in Cambridge, London, Ljubljana and Sydney. It has also started to win international awards including the ‘best AI product in insurance’ at CogX 2019 for the second year running.

Aeneas says that the CDT

has given me useful intuition to design our current architecture at Cytora, where we handle thousands of documents per second in streaming mode... My courses in physics and mathematics, alongside the research experience from my PhD, have also made it easy for me to get up to speed with current research in artificial intelligence and natural language processing, which we use at Cytora.

A notable feature of these companies is that the student leaders have recruited others in our CDT to provide expertise to deliver their products, demonstrating the direct influence of our CDT in supporting these entrepreneurial activities. The CDT has been supportive of the

⁴⁰ <https://cytora.com/>

students involved, offering flexibility to balance their studies and entrepreneurial activities. Fabian Renn-Giles writes,

My entrepreneurial endeavours were welcomed by all of my supervisors and always taken into account when planning the timeline of my PhD - for this I am hugely thankful. This is such a contrast to the way things were before I had joined the CDT.

In another example, the TSM-CDT facilitated Ben Kaube to take a break from writing up his thesis to work on his mobile phone app *TrainTrick*. Each year over 150 million passenger journeys are delayed in the UK. TrainTrick helped passengers hold train companies to account for delayed services by making it easy to claim money back. Launched in July 2016, TrainTrick has been featured on radio and TV and the Guardian newspaper voted TrainTrick one of the top 10 travel apps alongside Uber and CityMapper. Not surprisingly the train companies tried to shut down TrainTrick and eventually they succeeded in August 2017, but only after ‘qualifying delay thresholds have been halved for many commuters, compensation is now paid out directly, in cash rather than in vouchers and train company claim submission systems continue to improve’⁴¹.

Other entrepreneurial activities include:

- CrowdSense, an idea for collecting distributed sensor data for the sciences. The two students behind it, Fabien Renn and Niccoló Corsini, took part in a Digital Science Catalyst Grant competition hosted by our CDT and, as a result, were invited (with expenses paid) to SciFoo Camp at the GooglePlex in California. Niccoló has since founded a company Sonodot which ‘develops state-of-the-art indoor tracking technology

⁴¹ <https://tinyurl.com/spxneos>

that continually monitors the movements of material handling vehicles (for example forklifts) wherever they are in a factory. The Sonodot platform then reports this data to managers, allowing them to make better decisions around safety, human labour and fleet utilisation’⁴².

- Reroo is a mobile phone app that finds ‘alternative indirect train routes to show the user the cheapest options available, as well as the most direct and fastest train routes’⁴³. It was co-founded by Tom Edwards and was the winner at the HackTrain hackathon held in March 2015⁴⁴.

As noted by our IAB:

The range of transferrable skills courses on offer by the CDT is excellent. All courses on offer train students in a useful range of skills in addition to their scientific research.

In combination with our core training in computational methods and software development, this has helped nurture the entrepreneurial successes of our students.

6.1.5 CS5: Student leadership - Hermes

Hermes is a biennial summer school⁴⁵ held at Cumberland Lodge in Windsor Great Park. Its aim is to combine world class science and science communication in a school organised by students, for students. Around 50 postgraduates in TSM from all over the world are selected to attend. They include students from developing countries such as

⁴² <https://www.sonodot.com/>

⁴³ <http://reroo.co.uk/>

⁴⁴ <https://tinyurl.com/r9fthqj>

⁴⁵ <http://hermessummerschool.org/>

Argentina, Brazil, Chile, India and South Africa with sponsorship from organisations including Unilever, the Thomas Young Centre, Wolfram and CECAM. The format of Hermes is a series of masterclasses on TSM and science communication, given by internationally renowned experts, followed by the challenge of producing short videos to communicate the contents of the masterclasses to a general audience.

The first Hermes Summer School was held during the London 2012 Olympics and was the brainchild of Julian Walsh. In the run-up, and in collaboration with the Royal Society of Chemistry (RSC), the organisers launched an international outreach campaign aimed at fostering a mutually useful and respectful dialogue between scientists and the general public. Based on the so-called Mpemba effect, or ‘Why does hot water sometimes freeze faster than cold water?’ the RSC-Hermes challenge attracted over 22,000 submissions from amateur scientists around the World. The success of the campaign created significant media exposure for Hermes 2012 and its sponsor organisations with interviews with the co-chairs on the BBC Radio 4 World at One programme and Channel 4 News and coverage by the online and print editions of *The Guardian*, *The Daily Mail* and *The Daily Telegraph*.

Hermes 2012 left an enduring legacy and every two years since then students of the TSM-CDT have organised another Hermes event. Previous materials modelling masterclass speakers include: Prof Nicola Spaldin (ETH Zurich), Prof Craig Carter (MIT), Prof Kurt Kramer (Director of Polymer Theory, MPI-Mainz), Prof Sharon Glotzer (University of Michigan), Prof Peter Gumbsch (Director, Fraunhofer Institute for Mechanics of Materials), Prof Mark Miodownik (Director, Institute of Making, UCL), Prof Nicola Marzari (EPFL) and Prof Vasek Vitek (University of Pennsylvania). These technical classes are complemented by talks on science communication, which have been delivered by experts including: Piero

Vitelli from island41.com, Dr Simon Foster (CDT Outreach Officer), Gareth Mitchell from the Science Communication Group at Imperial, and Adelina Chalmers, an award winning professional speaker and CEO of Presenting Good Practice.

Feedback from Hermes has been overwhelmingly positive. Professor Craig Carter from MIT wrote:

I am deeply impressed with what you have accomplished... With profound admiration for what you have given the community.

Lucile Dézerald then at CEA Saclay, France wrote:

I can't find the words to say how much I loved this workshop, I learned so much and had so much fun.

Swastibrata Bhattacharyya from the Indian Institute of Science in Bangalore wrote:

Cheers to the organizing team. It was a nice work and you have inspired me a lot. Still can't imagine how students could arrange such a big event.

Nikoletta Prastiti, TSM-CDT student, wrote:

We were so thrilled by this incredible event that we were led to create a team of volunteers and initiate the procedures for organising Hermes 2018. We are very much looking forward to it!

Hermes is one example of how our CDT empowers students and strengthens their confidence and organisational skills.

6.1.6 CS6: Student outreach activities

Research in our CDT addresses some of the fundamental challenges society is currently facing in areas such as energy, transportation, communication and healthcare. To inform the public about our research, our CDT has developed a highly successful outreach programme. Activities include:

- The INSIGHTS work experience programme, where a group of A-level students are placed in our CDT and learn about its structure from administrator to lecturer.
- The INSPIRE teacher training programme, which aims to bridge the gap between university research and school science and mathematics by training teachers in a university environment.
- The Women in Physics event, which exposes approximately 200 female students in years 10-12 to the frontiers of physics research each year.
- The W12 festival 2016, where our CDT students engaged the local community of Imperial College's White City Campus in science experiments.
- The African School on Electronic Structure Methods and Applications (ASESMA) 2015 in Johannesburg, South Africa, where our CDT students organized hands-on training sessions on state-of-the-art electronic structure methods for 41 students from 10 African countries.
- Departmental Open Days, most notably the Physics Open Day 2016 where our CDT student Adam Ready demonstrated the power of supercomputers to prospective students by solving the Tower of Hanoi problem using a self-made cluster of Raspberry Pi computers.

In 2017 two of the five Imperial College President's Awards for Excellence in Societal Engagement⁴⁶ were given to our students. One went to Beth Rice who is the founder, organiser and architect of a Science Club for girls aged 6 to 11 that runs at the Baytree Centre in Brixton. This is a charity set up during the social unrest of the 1980s as a safe space for girls and women to develop socially and educationally.

The goal of this club is to encourage girls to develop an interest in science and to develop scientific thinking. For this, Beth focuses on do-it-yourself, home science experiments designed to introduce girls to scientific ideas and to encourage them to be curious about the world around them. Due to the success of the Science Club for the 6-11 age group, Beth has started a second Science Club for the 11-13 age group, which has proven equally popular. Through her work, Beth is supporting, encouraging and educating girls from some of the most disadvantaged neighbourhoods and schools in south London.

The second award went to Chris Ablitt and Rob Charlton who were the key organisers of the 'Atoms to Galaxies' series of the Pint of Science Festival. Pint of Science is an annual event that aims to bring cutting-edge research to the public in an accessible format and in the relaxed atmosphere of a pub. Chris, Rob and their team attracted sell-out crowds of over 100 people every night it ran. Miriam Ries who was Imperial's coordinator for Pint of Science in 2016 wrote that the event ...

was very successful. Particularly the hands-on demonstrations really made it stand out as a special Pint of Science event and were very engaging for members of the public. I attended on one of the nights and one of the speakers the CDT students had recruited even brought along a drone! It was a pleasure working with Rob and Chris, who were my main points of contact within the team organising 'Atoms to Galaxies'

⁴⁶ <https://tinyurl.com/qnu525j>

and I am very thankful for their hard work, as well as that of the other team members and additional volunteers helping out on the night.

In every year since the creation of the Pint of Science Festival in 2012 various students from our CDT have been involved in organising at least one of the Imperial events. In 2016, the festival took place in approximately 100 cities in 12 countries across 5 continents and was awarded the Points of Light Prize by Prime Minister David Cameron.

In 2018 our CDT students engaged with the public at the Royal Society Summer Science Exhibition at a stand entitled ‘Code for Creation’. This is one of the most prestigious science exhibitions in the country, attracting thousands of visitors of all ages and the media throughout a week in July. Students developed and presented four exhibits at the stand.

The TSM-CDT empowers and encourages its students to carry out outreach events and engage the public. This is achieved through the training provided by the CDT Outreach Officer Dr Simon Foster, the Science Communication course in year 3 and our CDT Student Prize for Outstanding Contributions to Outreach. The cohort-based approach of our CDT is a crucial factor for the success of outreach activities as it greatly facilitates the formation of small groups of students who share the additional responsibility of organising outreach events. The success of the stand at the Royal Society Summer Science Exhibition was a direct result of such collaboration.

6.2 The outcome of the 2017 mid-term review

On March 7, 2017 EPSRC informed the CDT Director, Dr Arash Mostofi, that the TSM-CDT was judged by the Oversight Panel to be in the highest of four assessment categories. On April 24, 2017 our CDT received the following feedback:

EPSRC believes that this CDT is performing very strongly and that there is much the team could do to guide and help the leaders of the other CDTs to help with adoption of best practice. EPSRC would particularly like to comment on the clearly demonstrated added value of the CDT, with respect to cohort building and especially the ongoing transferable skills training and also with respect to the widespread network of resulting research collaborations. Whilst this added value aspect is almost obvious to the CDT management team, their activities significantly exceed those of many comparable CDTs. EPSRC has also been particularly impressed with the professional approach taken to the governance and management of this CDT and note the effectiveness and level of engagement of the IAB. The Oversight Panel expressed some concerns about unfulfilled promises from collaborating companies despite the best efforts of the CDT team.

Going forward, EPSRC would like to see strong institutional support for Dr Mostofi, in order to enable him to grow as the CDT director and take ownership of its activities and future direction.

Arash had become the CDT Director only a few months before the submission of the 2017 mid-term review documentation. He received institutional support through his promotion to Professor on September 1, 2018. He also set up a ‘CDT strategic advisory team’ comprising the preceding director Professor Peter Haynes and me.

The TSM-CDT established strong collaborations with other companies that more than compensated for the ‘unfulfilled promises’ from a few of our industrial collaborators. Innovations introduced by the TSM-CDT such as the cohort mentor scheme, had already been shared with other CDTs and had formed the template for the College-wide mentor scheme. The highly acclaimed Career Planning Course has been shared with other CDTs within and beyond Imperial. The format of our interviews of candidates to join the TSM-CDT has been shared with other CDTs at Imperial as an example of best practice.

Commenting on the feedback from EPSRC the Provost of Imperial College, Professor James Stirling, wrote the following:

It really is tremendous to hear about feedback like that from such a key partner as EPSRC - such glowing words really are testament to the hard work of everyone involved.

Given:

- this exceptional feedback from EPSRC,
- our strong national and international reputations for excellence in education, training and research,
- the outstanding quality of our students,
- the high value our industrial collaborators attached to our research and our students,
- the high level of funding we were attracting from our industrial partners,
- our constant search for ways to innovate and improve the student experience,

given all that we felt we were in a strong position to apply in 2018 for a further 5 years of funding for the TSM-CDT from EPSRC.

7. The EPSRC call for outline CDT proposals in 2018

EPSRC issued the call⁴⁷ for 4-page outline proposals for CDTs on January 17, 2018, with a closing date of March 13, 2018. Successful outline proposals would lead to invitations to submit full proposals later in 2018. This was our second bid to renew the funding for the TSM-CDT for a further 5 years. It would provide a further 5 cohorts, amounting to at least 50 students, with the first cohort starting in 2019 and the last cohort finishing their 4-year PhDs in 2027. The fees and stipends of at least 10 studentships in the 5 cohorts had to be funded from sources other than UK research councils.

EPSRC summarised the objectives of the call as follows:

- to ensure a forward-looking, ambitious portfolio of research training which makes a positive difference for the UK.
- to protect the UK's long-term capability and foster an expansion of multidisciplinary research.
- to secure leverage in order to maximise the benefit of public funds.
- to train the next generation of UK leaders for industry, research organisations and elsewhere.

The call had two funding streams:

⁴⁷ <https://tinyurl.com/rhah53v>

- A priority area stream - for proposals delivering against priority areas articulated within the call. This stream was allocated 70% of the available funds.
- An open stream - for proposals in areas outside the identified priorities, but still predominantly within the remit of the research council, which are best delivered through a CDT approach. This stream was allocated 30% of the available funds.

The call stated that applications from existing CDTs will be treated equally with those for new CDTs, and that they will all be assessed using the same assessment process and criteria. It also stated that there will be no expectation on the number of existing or new Centres that will be supported. The following statement also appeared in the call:

Information about existing centres will not be made available to peer review by EPSRC; this includes the outcome of the mid-term review exercise.

Considering the very detailed information in the mid-term review (all 36 pages of it – over half the length of this book) was collected only 12 months before the call was issued it is hard to fathom why peer review was denied access to it. The 2017 mid-term review was also not mentioned in the later call for full proposals.

The three equally weighted assessment criteria were as follows:

1. National need for cohort-based doctoral training.
2. Centre vision and leadership.
3. Quality of the research training environment.

Finally, unsuccessful applicants would receive no feedback.

The first decision Arash, Peter and I had to make was to which stream to apply. This was not an easy decision as none of the priority areas suited us as well as in the previous round of applications in 2013 where the priority area ‘Computational and Theoretical Physical Sciences’ was a good fit for our CDT. After some discussion we chose the 15th in the priority area stream: ‘Mathematical and computational modelling’. This was certainly the best fit for our CDT, but we were concerned about its breadth, although we felt our track record should stand us in good stead. However, we realised it would be very unlikely there were any members of the peer review panel who had knowledge of or interest in TSM.

Arash then drafted the 4-page outline proposal addressing the three assessment criteria. Peter Haynes, Johannes Lischner (Deputy Director) and I carefully reviewed successive drafts and made suggestions for improvements. We all agreed the final draft and we all shared responsibility for it. The Vice Deans of Imperial read all the outline proposals from the College, paying close attention to the three assessment criteria. Arash was told informally that our outline proposal was among the top few of about 50 outline proposals in Imperial. Our proposal was submitted by the College to meet the EPSRC deadline of 4pm on March 13, 2018.

We found out on May 30, 2018 that our outline proposal was unsuccessful.

Our CDT will cease to exist in October 2022 when our tenth cohort of students complete their PhDs.

7.1 Aftermath

The only feedback we received from EPSRC was the following non-specific text:

General feedback: The Panels recognised that many existing centres were currently providing high quality doctoral training. However, feedback from across all the outline CDT panels was that some existing centres, whilst providing evidence of ability to deliver high quality training, were weaker at demonstrating the continued and future need for a CDT and the training that it will provide.

To demonstrate that this feedback is completely inapplicable to our outline proposal I quote here the entire section that addressed the first assessment criterion:

1. National need for cohort-based doctoral training (quoted from our outline proposal of 2018)

The mission of this EPSRC CDT in Theory and Simulation of Materials (TSM) is to create a new generation of scientists and engineers with the theoretical and computational abilities to tackle complex, real-world problems in materials science and engineering that span traditional boundaries between disciplines. Building on an established programme, this CDT will address the critical shortage of trained researchers capable of generating physically-based, predictive models of phenomena and processes in materials across a range of length and timescales and who have a deep appreciation of industrial and experimental context.

Materials underpin every modern technology, including energy conversion and storage, transportation, electronic and optical devices, environment, defence and healthcare. Advances in materials often dictate the pace of technological progress and major knowledge economies recognise materials as an important strategic priority

*essential for underpinning key areas of high value manufacturing, as well as addressing a range of important societal ‘grand challenges’ in areas such as mobility, healthcare and energy.*⁴⁸

The impact of materials on the UK economy is correspondingly significant. A report by the Royal Academy of Engineering⁴⁹ noted UK businesses that produce and process materials are worth £197bn/year. The UK has invested heavily in world-leading materials research and translation initiatives such as the £235M Henry Royce Institute to accelerate the use of advanced materials in existing and emerging industrial sectors (Imperial is a founding partner), and the £1bn Industrial Strategy Challenge Fund, with £272M so far to develop battery materials and technology (Faraday Challenge) and materials for future manufacturing.

The capability to predict material properties and understand fundamental mechanisms using computational tools based on physical principles has established TSM as an indispensable pillar of contemporary materials research that is complementary to experimental investigation. In a recent study⁵⁰, 80% of companies surveyed reported innovation accomplishment, 60% cost savings, 35% job creation and 30% revenue increase as a result of TSM, with an average reported return on investment of a factor of 8. In the US, the DoE has recently invested \$48M in the creation of five new Centers in Computational Materials⁵¹ and, in the EU, the European Materials Modelling Council has the goal for *materials modelling and simulation [to] become an integral part of product life cycle management in*

⁴⁸ A Review of International Public Sector Strategies and Roadmaps: A Case Study in Advanced Materials (2014), p. V. <http://bit.ly/2BQzSST>

⁴⁹ Innovation in Materials (2014), p. 3. <https://tinyurl.com/suceeby>

⁵⁰ G Goldbeck & C Court, The Economic Impact of Materials Modelling (2016). <https://zenodo.org/record/44780>

⁵¹ <https://tinyurl.com/sj6grpl>

*European industry, thereby making a strong contribution to enhance innovation and competitiveness on a global level.*⁵²

As an underpinning activity, TSM lies principally within the *Mathematical and Computational Modelling* priority area, but its applications span many other areas. From EPSRC's Balancing Capability Exercise⁵³, five out of twelve *grow* areas and over twenty *maintain* areas are represented in the current portfolio of TSM-CDT research projects, including Software Engineering, Materials for Energy Applications, Energy Storage, Biophysics & Soft Matter, Continuum Mechanics, Materials Engineering and Light-Matter Interaction.

The growth in usage of TSM is evidenced by the success of the web portal nanoHUB.org, which offers users a wide range of materials simulation tools. There are currently 17,000 users of these tools, compared to only 6,000 ten years ago; 1,714 papers cite nanoHUB.org resources, 258 of which (6.4%) are by authors in industry⁵⁴. The portal also highlights the demand for training in TSM: there are over 12,500 students enrolled in short online courses provided through the nanoHub-U platform, 10% of those from industry.

It is clear that training in TSM is a critical issue. Separate disciplines act as silos of knowledge, each specialised in phenomena and processes at a particular length- and/or time-scale and each with its own approach and language. For example, in physics and chemistry, the focus is typically on electronic and molecular phenomena, whilst in engineering it is more on continuum level descriptions at a component level. In practice, however, most problems in materials science and engineering involve multiple scales that are strongly coupled and the intellectual and language barriers between disciplines must be overcome to bridge

⁵² <https://tinyurl.com/quvyyc9>

⁵³ <https://tinyurl.com/wa8j68r>

⁵⁴ slide 9 of <https://tinyurl.com/qrlnnk2>

scales and arrive at integrated cross-disciplinary solutions. No undergraduate programme anywhere in the UK covers the range of disciplines and skills required to achieve this. Moreover, transformative research in TSM often requires innovation in theoretical models and simulation methods, and hence software, but undergraduates from most physical sciences and engineering domains have limited literacy in the fundamentals of software engineering, numerical methods, high-performance computing and handling large data sets. As noted recently,

*... the greatest challenge looming is an educational one. Simulation science ... requires a steady mastery of the fundamentals of condensed-matter physics, statistical mechanics, physical chemistry and materials science, supported by the knowledge of applied-math numerical techniques, advanced programming models and ever evolving computer architectures. Traditional departments are far away from offering this focus and this mix and so there is both the opportunity and the urgent need for education models that focus on twenty-first century polymaths.*⁵⁵

The TSM-CDT aims to address this growing need. A cohort-based approach is ideal because it enables the integration of expertise from many domains to deliver the training programme. It encourages collaboration among students, who arrive with a range of disciplinary backgrounds and helps them to combine their strengths to solve a greater range of problems than would be possible otherwise.

Demand for the course from students is high, with an average 56 serious applicants per cohort, notwithstanding the normal requirement of a first-class degree in physical sciences, engineering or mathematics.

⁵⁵ Materials Modelling: The Frontiers and the Challenges, Nature Materials **15**, 381 (2016). <https://www.nature.com/articles/nmat4613>

We have also witnessed strong demand for the combination of skills that our graduates develop in the CDT. Prof Boris Kozinsky (Harvard), formerly Principal Scientist of Bosch Materials Theory and Simulation in Boston, writes

The [TSM-CDT] students' training in theory and simulation of materials, computational methods and collaboration skills is an excellent preparation for the environment at Bosch Research where our work is application-driven and demands creative practical problem solving. The two students we hosted also taught us a great deal and were easily among the best we have had in terms of motivation, productivity and impact ... I wish there were more centers that offer this level of preparation.

Demand from employers for TSM-CDT graduates is also high: over half enter TSM-related industries (including with our partners Rolls-Royce, CCFE and Materials Design) or in industry sectors where their problem-solving, software and data analysis skills are keenly sought (including IBM, Cisco Systems and HMRC); and 40% continue to use their skills in academia, including postdoctoral positions at MIT, UC Berkeley and Harvard as well as three prestigious independent fellowships. There are also examples of successful entrepreneurs, including Dr Aeneas Wiener, founder and CTO of Cytora⁵⁶, a company that monitors openly available sources of information to assess geopolitical risk, and Dr Ben Kaube who founded newsflo⁵⁷, a provider of bespoke media monitoring for universities.

The TSM-CDT has initiated culture change towards multi-disciplinary research by requiring all projects to have two supervisors with complementary expertise at different scales. This is evidenced by

⁵⁶ <https://cytora.com/>

⁵⁷ <https://www.elsevier.com/en-gb/solutions/newsflo>

the evolution of the network of cross-disciplinary collaborations, which has spread to over 80 supervisors from nine Imperial departments and 17 partner organisations. In this proposal we seek to build on this impact and drive further culture change by aligning TSM-CDT research projects with industry-motivated scientific and technological challenges that require: (1) bridging fundamental science and engineering through the development and use of physically-based models; and/or (2) exploiting the convergence of scales accessible to both TSM and experimental characterisation through collaboration with researchers at experimental facilities and other experimentally-led cognate CDTs. This new emphasis will accelerate the vision for an integrated approach to materials innovation in industry, as embodied in the UK's Industrial Strategy. At the same time, we will further our commitment to innovation in training by: working with students and partners to revise the design and delivery of the training programme; providing more opportunities for cohort-based group projects involving partners and interactions between cohorts and with cognate CDTs via the national network of CDTs associated with the Royce Institute; and leveraging our growing network of alumni to inspire new cohorts of students.

End of quotation for our outline proposal of 2018.

The decision not to renew the funding of our CDT has been met with dismay by our industrial partners and by researchers involved in TSM around the World. An author of an outline proposal in direct competition with ours, commenting on the decision to axe our CDT, wrote:

I find this incomprehensible and it seems to me to be a decision that is wantonly destructive of an extremely strong part of the UK's research capability. This will leave members of the UK's modelling community, wherever we are based, in a much worse position.

It turned out that ours was not the only highly valued CDT Rolls-Royce had lost at the outline proposal stage. Dave Rugg said the Corporate Group of the company sent an 'extremely robust formal response' to EPSRC, followed by a face-to-face meeting to try to get the 'extremely disappointing decisions' reversed. In reply EPSRC said the decisions were irreversible.

Other members of our IAB wrote letters to John Hand, Physical Sciences Lead at EPSRC, to try to get the decision reversed. Here is a selection from their letters.

Dr Erich Wimmer, Chief Scientific Officer and Chairman of the Board of Materials Design Inc., which is an SME, wrote:

I am utterly amazed that the TSM-CDT proposal from Imperial College has been dismissed and I am urging you to review this decision and to allow it to proceed to a full proposal stage.

There are three important reasons why this proposal should be reconsidered, namely

- 1. The TSM-CDT addresses an area of utmost strategic importance, namely educating and training the next generation of leading scientists and engineers to develop and reap the full benefits of computational materials science and technology. This technology will be a key competitive factor in the 21st century.*
- 2. The TSM-CDT has over the course of 10 years developed a world-leading reputation for outstanding technical and*

professional training, research, industry engagement and a deep commitment to its students.

- 3. The research groups involved in the TSM-CDT consist of world-renowned scientists in their fields, thus offering unique quality to their students. Let me add two more personal comments. Our company, Materials Design, has had excellent experience with students who graduated from the TSM-CDT or worked as interns as part of their doctoral programme. In fact, as a provider of highly sophisticated computational materials science software we are witnessing the dire need of industrial R&D groups for well-trained scientists and engineers in the field of computational materials science. This TSM-CDT is exactly addressing this need.*

As I am writing these lines, I am returning from the Far East. It is obvious that especially China, Japan, Korea and Taiwan are massively investing in advanced research in the field of computational materials science whilst the West is in serious danger of falling behind. This would be particularly tragic as most of the current technology in the field of computational material science has its roots in the West. Thus, it is of utmost importance to keep building on successes such as the present TSM-CDT. In this context, I urge you to review the decision on the above proposal.

Professor Sergei Dudarev, Head of the Materials Modelling Group at CCFE, wrote:

I am writing to express our deep concern about the decision by EPSRC not to invite the CDT on Theory and Simulation of Materials (TSM-CDT) at Imperial College to submit a full proposal to renew its funding for another 5 cohorts of students from 2019.

A key aspect of the research we do at CCFE/UKAEA concerns the simulation of defect microstructure created by irradiation in metals and alloys. This research is fundamental to reactor design and the safe and efficient operation of fusion or fission nuclear reactors. The work involved is highly mathematical and it also requires a thorough understanding of the physics of defects and complexities of their interactions over a wide range of length and time scales.

Over the past 8 years we have benefitted from a close collaboration with the TSM-CDT. We have been directly involved in the joint supervision of the PhDs of some truly outstanding young scientists from the TSM-CDT. These collaborations have resulted in world-leading, ground-breaking research, which has propelled the UK to the forefront of this area of physical materials science. This has been made possible primarily by the exceptional quality of the students that the TSM-CDT attracts from Physics departments in the UK and Europe and the unique quality and depth of education, training and mentoring they receive in the TSM-CDT. We are not aware of any other university in the UK with the capability to deliver education, training and research supervision of comparable quality in this area.

It is our hope that the decision not to allow the TSM-CDT to submit a full proposal will be reviewed, to allow it to compete for the renewal of its funding by submitting a full proposal.

W Craig Carter, POSCOE Professor of Materials Science at MIT wrote:

I was dismayed to learn of the EPSRC decision not to allow the CDT on Theory and Simulation of Materials to submit a full proposal for a further 5 years of funding from 2019. The news came as a shock - I can't imagine that the TSM-CDT could be considered anything other than a model of success.

I've been following this CDT from its very beginning and am a great fan - in fact, envious - of what they have achieved since 2009. I've been a member of the TSM-CDT's board of advisors since its beginning.

I have been a Professor of Materials Science at MIT for about 20 years, published nearly 200 papers and a well-known textbook, co-founded a renewable energy company (24M). I've won every teaching award at MIT as well as some from scientific societies and I am very interested in the science of technical education. I have been invited to all four of the HERMES conferences that the TSM-CDT students have organized and will attend again this summer. I am a theoretical and computational materials scientist and very familiar with the research that is being performed at the TSM-CDT.

From my perspective, from its beginning in 2009 with Adrian Sutton, continuing with Peter Haynes and now in the able hands of Arash Mostofi, the center has been the model of excellent education and training. They have produced students who have gone to industry, created their own start-ups, joined service organizations and have gone into academia. In addition to academic research, they were producing research that was being employed by Rolls-Royce and many other UK industries. All of these efforts serve as a great benefit to the UK and other economies and for a technically trained future workforce. It seemed to me that the TSM-CDT was doing exactly all that was envisioned when the CDT program was created by the EPSRC. In my opinion, the team of 80 researchers across 9 departments at Imperial and the outstanding students the CDT recruits, produces research of a unique breadth and world-leading quality. This group is widely recognized as being the best in the world. Many other CDTs were adopting best practices from the TSM-CDT including the cohort mentor scheme, their procedures for interviewing students for admission into the CDT, and their acclaimed careers planning courses.

Thus, I was perplexed when I heard the distressing news that the EPSRC would not continue its support.

The research performed at the TSM-CDT was and is fresh and exciting. So many interesting things are coming out of the multi-disciplinary interactions at Imperial and the collaborative research with industry. Elsewhere, students are not encouraged or equipped to develop new theory and new computational techniques to address current challenges, but to use a very limited set of standard computational techniques as black boxes. By contrast TSM-CDT students receive training in the art of taking real industrial problems in all their complexity and translating them into scientific hypotheses that can then be explored and tested theoretically and computationally. This requires imagination, theoretical insight and an ability to listen to partners in industry facing technical challenges. It goes to the very heart of what it means for academics to work with industry. This full engagement - to understand and address industrial materials challenges - is what sets the TSM-CDT above any other theoretical materials group in the world.

The fundamental goal of the TSM-CDT was impeccable: give students a broad research experience by cooperative advising across disciplines and give them superb educational fundamentals. I have never encountered more enthusiastic, well-trained and highly performing students over the almost 10 years that I have been associated with the TSM-CDT. Beyond this training, the students were learning important leadership and professional skills - the exposure to these skills was crafted by the administrative leadership of the TSM-CDT and the students were enthusiastically absorbing such skills. I am confident that many of these students will be in leadership positions in the UK.

... Frankly, I was and am envious of what Adrian, Peter and Arash created. If I had been able to convince NSF to support a similar

educational enterprise, I would have been very pleased. The disappearance of the TSM-CDT will be a sad loss and perhaps a catastrophic dismantling of a bona fide UK national resource. I believe that - with future hindsight - the loss of the TSM-CDT will be seen as an unfortunate mistake.

I am not sure what happened. It is often the case proposal reviewers will look for novelty or fads; it is sometimes the case that they will try to redistribute resources. However, it is less often the case that a reviewer will recognize extant excellence and support continuing that. I believe this CDT has done everything the EPSRC envisioned.

There were other letters in a similar vein from our industrial partners. They all expressed their shock and disappointment at the decision.

By coincidence the IAB met a few weeks later on June 20th, 2018. John Hand, Physical Sciences Lead at EPSRC, agreed to attend the meeting. It could not have been a comfortable meeting for him and we appreciated his attendance. One after another members of the IAB made clear to him their dismay at the decision taken by EPSRC not to allow us to proceed to full proposal. But since it was made by “peer review”⁵⁸, he explained, EPSRC was unable to reverse it. John wanted to explore whether the TSM-CDT could be rescued by some other means. He was eager to see whether a combination of our strong financial support from industry and a contribution from the College may enable the TSM-CDT to survive.

The two critical factors were the cost of the teaching of the MSc and maintaining our healthy mix of industrial and blue skies research projects. We regarded both as absolutely essential to everything the TSM-CDT was about. The IAB members from industry said they were willing to double their financial contributions to support the TSM-

⁵⁸ I have put peer review in inverted commas because it is unlikely our proposal was reviewed by people with expert knowledge of TSM or even interest in it.

CDT. But they could not pay for the MSc, nor would they pay for blue skies research projects. We knew there was no point in asking Imperial to pay for them either. No top university in the UK will pay for the small group teaching we were delivering in the MSc. A top UK university will pay for blue skies research projects only through a small number of scholarships in open competition across the university. Without EPSRC funding the TSM-CDT cannot continue.

7.2 Where are we now?

The last cohort to undertake the MSc in our CDT finished it in September 2019. Education and training in the UK in theoretical and computational materials science has returned to the parlous state I described in the proposal I wrote in 2008 (see section 4.1). Our industrial partners and other companies no longer have access to the research our CDT was able uniquely to provide or to recruit our graduates. I do not believe there is another university in the UK capable of delivering the MSc course and the research environment our CDT provided. There can be no doubt that we have lost ‘an extremely strong part of the UK’s research capability’.

8. Final thoughts

8.1 EPSRC

Peer review is imperfect. But it is undoubtedly the only acceptable way to decide which proposals to fund. Given that the peer review panel was almost certainly not expert in TSM and that EPSRC denied the panel access to the comprehensive 2017 mid-term review submissions and results, their decision about our CDT is not surprising. But in the 2018 round of applications our CDT was not the only top-rated CDT to be axed.

In the mid-term review of 2017 there were 44 top-rated CDTs, of which 28 were cut in the 2018 round of applications according to Michael Banks' analysis⁵⁹. Even more surprising is that some of the lowest rated CDTs in the mid-term review of 2017 *were* funded again in the 2018 round.

In the absence of meaningful feedback from EPSRC it is impossible to understand how these shocking decisions were reached. However the decision to axe our CDT was reached, it does not sit comfortably beside the EPSRC mission statement⁶⁰:

[To] advance knowledge and technology ... and provide trained scientists and engineers, which meet the needs of users and beneficiaries..., thereby contributing to the economic competitiveness of our United Kingdom and the quality of life.

John Hand expressed his concern at the IAB meeting on June 20, 2018 that there was a significant number of other top-rated CDTs that were axed at the outline proposal stage. But the situation only got worse

⁵⁹ Michael Banks, *Physics World*, March 2019. <https://tinyurl.com/vm24e7u>

⁶⁰ <https://epsrc.ukri.org/about/facts/mission>

at the full proposal stage, after which it appears that 28 top-rated CDTs in all were axed. This is a disaster, not only for those top-rated CDTs, but for UK science and engineering and the UK plc.

Rolls-Royce accounts for 0.7% of GDP and 2% of all UK goods exported. It employs 22,000 people in the UK and supports approximately 135,000 British jobs⁶¹. I suggest that a company of such importance to the UK economy, that has invested so much time and money in supporting our CDT, should have been consulted in the decision about the future of our CDT. After all, EPSRC demands that a significant fraction of the funding for a CDT, equivalent to at least 10 studentships, comes from sources other than research councils. EPSRC is not the only stakeholder in a CDT.

8.2 The future

In September 2019 I was invited to spend 3 delightful days at MIT. They asked me to give a lecture describing our CDT, about which they had heard a great deal. MIT had recently received a very substantial donation from a private donor and they were thinking about launching a major initiative on TSM. In my talk I focused on the student experience in our CDT, stressing how different it was from the traditional PhD experience. I spoke less about our research because the audience already knew it was of a very high quality. When I reached the last slide I said we were having to hand on the baton to MIT because EPSRC had decided not to renew our funding for a further 5 years. There were gasps from the audience.

In the discussion after my lecture I was particularly struck by two comments from the audience. The first was that my talk had ‘highlighted the fickleness of funding from the state’. It had certainly felt very fickle to me. The second comment was from Professor Sidney Yip, from whose letter of support for the proposal I wrote in 2008 I

⁶¹ <https://tinyurl.com/wwu3gtx>

quoted in Chapter 4. He asked me to write down what we had done in our CDT so that others could benefit from it. His comment is partly why I decided to write this book.

If MIT does decide to launch an initiative on TSM I hope I may be involved in some way. In the UK I fear that education and training in TSM will now swiftly return to the primordial state it was in before 2009, with physicists graduating with PhDs in TSM knowing everything about nothing in materials science and materials scientists reaching for the nearest black boxes. Our CDT is winding down and by October 2022 it will cease to exist. It is quite possible that some of the key people at Imperial who made our CDT such a tremendous success will move on in the next few years. Perhaps to MIT?

It is possible the decision to axe 28 of the 44 top-rated CDTs in the 2018 round of applications will affect the success of the currently funded CDTs. It takes passion, hard work and commitment to make a CDT successful. The 2018 round has shown that EPSRC is willing to cut the funding, even after it has recognised a CDT is performing well, without explanation. That is unlikely to encourage a director to work flat out to make a success of their CDT. EPSRC's fickleness may also affect the willingness of companies to invest in growing a CDT.

In my view the best CDTs have led the World as models for PhD education and training. EPSRC deserves credit for pioneering them in the UK, often in the face of considerable criticism. But CDTs are too valuable for the scientific reputation and economic prosperity of the UK to be left in the hands of an organisation that has made such damaging decisions for UK science and engineering without even having to account for them.

8.3 Mitigating risk of future disasters: a different way

I have shown that continuation of funding from EPSRC is not guaranteed even if all its criteria for funding are met in full and the CDT is recognised internationally as being outstanding. The Achilles heel of our CDT was our critical dependence on funding from EPSRC for teaching in the MSc and for blue skies research projects. The weakness of the EPSRC process to review the outline proposals in 2018 was that the remit of the panel was far too broad for its members to have expertise in all areas of the proposals before it. It was also a crippling decision to deny panels access to the comprehensive information gathered in the 2017 mid-term reviews of existing CDTs. It was unfair to companies working with CDTs that they were not directly involved in the decisions about the futures of those CDTs. Is there a different way to mitigate the risk of losing outstanding CDTs?

One possible way might be to adopt a funding model for CDTs similar to that of the Max Planck Institute for Iron Research (MPIE) in Düsseldorf. The funding of this Max Planck Institute is unlike any other in Germany. A fraction of its funding comes from the Max Planck Society, which in turn gets its money from the Federal Government and the Federal States of Germany. The remainder comes from industry. But interestingly the funding from industry comes with no obligation on the MPIE to work on any particular industrial projects. The argument is that companies supporting the MPIE benefit when they recruit scientists the MPIE trains. More generally they benefit because the MPIE sustains an expertise relevant to those companies, which in turn sustains them. If those companies need specific research to be done they pay for it in addition to their standing annual charge. The MPIE is subject to a thorough review every 3 years, lasting 2 full days, by a panel of international experts from academia and industry. Some of the companies on the review panel are among those supporting the MPIE financially.

The MPIE has PhD students who are registered at local universities. Thus, the MPIE gives companies access to PhD graduates in areas relevant to them. That would not happen if the MPIE did not exist because those students would have to choose PhDs in other areas available in their universities.

In my view we should consider whether something similar to the MPIE model of joint funding by the state and the private sector could be established in the UK for CDTs. For example, I have highlighted the physics of metals as an area of exceptional importance for manufacturing industry, but which has vanished from physics departments in the UK. It is an area of physics that has become unfashionable on both sides of the Atlantic, despite its continued industrial importance. As our CDT has shown, it is an area that is rich in intellectually challenging and rewarding problems.

A CDT on metal physics jointly funded by the state and by manufacturing industry, along the lines of the MPIE model, would enable manufacturing companies to have continued access to expertise and people trained in metal physics. It would differ from the existing EPSRC funding model in that the split between state and industry funding would be more like 50/50. Also, the industrial ‘standing annual charge’ would be provided with no strings attached, as in the MPIE model. That would pay for the blue skies research. Specific industrial research projects would incur additional costs to the companies requesting them.

State funding would pay for the education and training, management and a negotiated number of student stipends for each CDT. It would be for academia and industry to work together to propose the themes of such CDTs, to ensure their relevance to existing and emerging industries and to ensure the themes are scientifically challenging and potentially rewarding. The number of such CDTs and the funding each

receives would not be determined by the state but by the demand from industry and academia working together.

Companies supporting the CDT would be involved directly in reviewing its performance and funding alongside other academic and industrial experts. This would be a more equitable way of involving industry in the funding decisions. It would also spread the risk by sourcing the funding from stakeholders who have a say in its continuation.