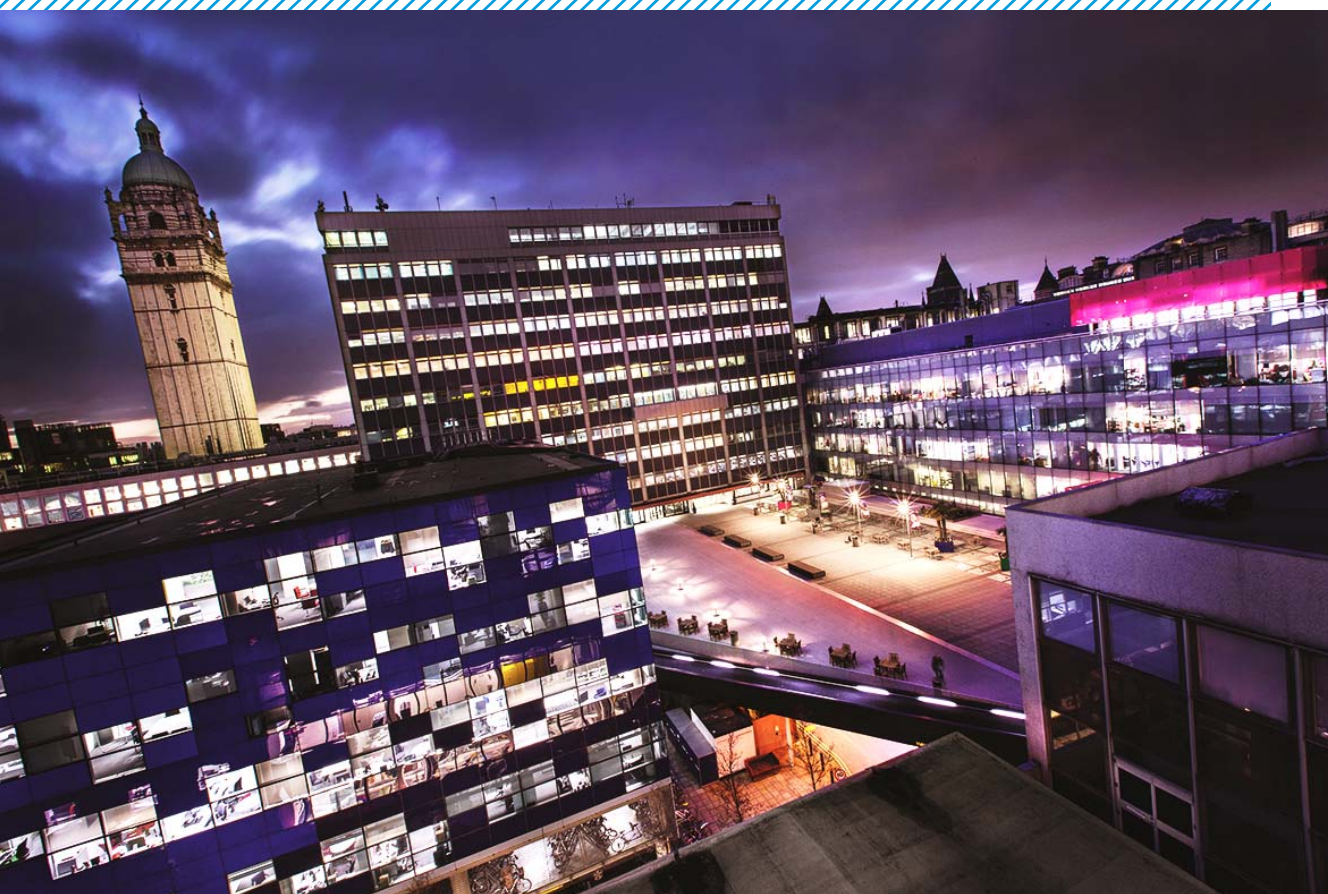


**Imperial College  
London**



**Faculty of Natural Sciences**

**Department of Physics**

**MSc in Theory and Simulation of Materials**

**STUDENT HANDBOOK**

**2018–19**

<b>Welcome to the College</b> .....	<b>5</b>
<b>Our Principles</b> .....	<b>6</b>
<b>Welcome from the Graduate School</b> .....	<b>7</b>
<b>The Graduate School</b> .....	<b>8</b>
<b>Welcome from the Graduate Students’ Union (GSU)</b> .....	<b>9</b>
<b>1. Introduction to the Department</b> .....	<b>10</b>
1.1 Welcome from the CDT Director .....	10
1.2 About This Handbook.....	11
1.3 Aims and Objectives of the MSc in Theory and Simulation of Materials.....	11
1.4 The Centre for Doctoral Training on Theory and Simulation of Materials .....	12
1.5 Academic and Administrative staff .....	13
1.6 Student Representation .....	<u>1415</u>
1.7 English Language Requirement.....	15
1.8 Attendance and Absence .....	15
1.9 Key dates 2018-19.....	<u>1516</u>
<b>2. Programme Information</b> .....	<b><u>1748</u></b>
2.1 Administration .....	<u>1748</u>
2.2 Timetables and the Working Day .....	<u>1748</u>
2.3 The Curriculum.....	<u>1819</u>
2.3.1 Overview .....	<u>1819</u>
2.3.2 Taught Courses.....	<u>1819</u>
2.3.3 Rapid Feedback Classes .....	<u>1920</u>
2.3.4 Computational Methods .....	<u>1920</u>
2.3.5 Industrial Engagement .....	<u>1920</u>
2.3.6 Literature Review .....	<u>1920</u>
2.3.7 Research Project.....	<u>1920</u>
2.3.8 Blackboard .....	<u>2024</u>
2.3.9 Outreach.....	<u>2024</u>
2.4 Imperial Mobile app.....	<u>2024</u>
2.5 Imperial Success Guide .....	21
<b>3. Assessment</b> .....	<b><u>2223</u></b>
3.1 Overview .....	<u>2223</u>
3.2 In Detail .....	<u>2324</u>
3.2.1 The Marks Available .....	<u>2324</u>
3.2.2 Schedule of Examinations .....	<u>2425</u>
3.2.3 Marking of Problem Sets .....	<u>2425</u>

3.2.4 Plagiarism .....	<u>2526</u>
3.2.5 Use of Materials for Teaching .....	<u>2627</u>
3.2.6 Use of Calculators in Written Examinations.....	<u>2627</u>
3.2.7 Written Reports.....	<u>2627</u>
3.2.8 Written Examinations.....	<u>2627</u>
3.2.9 Oral (viva voce) Examinations for Advanced Options .....	<u>2728</u>
3.2.10 Literature Review and Research Project .....	<u>2728</u>
3.2.11 Transferable Skills .....	<u>2728</u>
3.2.12 Letter Grades.....	<u>2829</u>
3.3 Requirements for Passing the MSc.....	<u>2829</u>
3.3.1 Classification of the MSc .....	<u>2829</u>
3.3.2 Progression onto Year 2 for CDT Students on the 1+3 year programme.....	<u>2829</u>
3.3.3 Resits.....	29
3.3.4 How To Complain .....	<u>2930</u>
3.4 Sutton Prize.....	<u>2930</u>
<b>4. Board of Examiners .....</b>	<b><u>3031</u></b>
4.1 Board of Examiners.....	<u>3031</u>
4.2 External Examiners.....	<u>3031</u>
<b>5. Location and Facilities .....</b>	<b><u>3132</u></b>
5.1 Location .....	<u>3132</u>
5.1.1 Maps.....	<u>3132</u>
5.1.2 Accessibility .....	<u>3132</u>
5.1.3 Smoke-Free Policy .....	<u>3132</u>
5.2 Facilities .....	<u>3233</u>
5.2.1 Admin Support.....	<u>3233</u>
5.2.2 Telephones.....	<u>3233</u>
5.2.3 Photocopying, Printing, Scanning, Office Supplies.....	<u>3233</u>
5.2.4 Mail .....	<u>3233</u>
5.2.5 Before you Arrive .....	<u>3233</u>
5.2.6 When you Arrive .....	<u>3233</u>
5.2.7 ID Cards.....	<u>3233</u>
<b>6. Working While Studying .....</b>	<b><u>3334</u></b>
<b>7. Health and Safety.....</b>	<b><u>3435</u></b>
7.1 Safety.....	<u>3435</u>
7.2.1 The College Safety Department .....	<u>3435</u>
7.2.2 Occupational Health Requirements .....	<u>3536</u>
<b>8. College Policies and Procedures .....</b>	<b><u>3637</u></b>
8.1 Regulations for Students.....	<u>3637</u>

8.2 Academic Feedback Policy .....	<u>3637</u>
8.3 Provisional Marks Guidance .....	<u>3637</u>
8.4 Late Submission Policy .....	<u>3637</u>
8.5 Academic Integrity.....	<u>3637</u>
8.6 Academic Misconduct Policy and Procedures .....	<u>3738</u>
8.7 Appeal and Complaints Procedures.....	<u>3738</u>
8.8 Student Disciplinary Procedure.....	<u>3738</u>
8.9 Intellectual Property Rights Policy.....	<u>3738</u>
8.10 Use of IT Facilities.....	<u>3738</u>
<b>9. Well-being and Advice .....</b>	<b><u>3839</u></b>
9.1 Student Space .....	<u>3839</u>
9.2 Departmental support and College tutors .....	<u>3839</u>
9.3 Advice Services.....	<u>3940</u>
9.4 Health Services.....	<u>4041</u>
9.5 Disability Support.....	<u>4142</u>
9.6 Library and IT.....	<u>4142</u>
9.7 Religious Support.....	<u>4243</u>
9.8 Support for International Students .....	<u>4243</u>
<b>10. Student Records and Data.....</b>	<b><u>4344</u></b>
<b>11. Work-life Balance.....</b>	<b><u>4445</u></b>
11.1 Imperial College Union.....	<u>4445</u>
11.2 Graduate Students' Union.....	<u>4445</u>
11.3 Physical Activity Sport.....	<u>4445</u>
<b>12. Student feedback and representation.....</b>	<b><u>4546</u></b>
12.1 Feedback from Students .....	<u>4546</u>
12.2 Student Representation .....	<u>4546</u>
12.3 Staff-Student Committee.....	<u>4546</u>
<b>13. Student Surveys .....</b>	<b><u>4647</u></b>
<b>14. And finally .....</b>	<b><u>4748</u></b>
14.1 Alumni Services .....	<u>4748</u>
14.2 Opportunities for Further Study.....	<u>4748</u>
14.3 And When You Leave Imperial.....	<u>4748</u>
<b>Appendix 1 Synopses of courses .....</b>	<b><u>4849</u></b>
Mathematics for the Theory of Materials (MTM1 and MTM2).....	<u>5051</u>
Equilibrium in Materials (EQM1) .....	<u>5152</u>
Transformations of Materials (TM1).....	<u>5354</u>
Electronic Structure of Materials (ESM1).....	<u>5556</u>
Classical Field Theory of Materials (CFTM1).....	<u>5758</u>

Methods of Simulating (MSM1 and MSM2) .....	<u>5960</u>
Equilibrium in Materials (EQM2) .....	<u>6263</u>
Transformations of Materials (TM2) .....	<u>6364</u>
Electronic Structure of Materials (ESM2) .....	<u>6465</u>
Classical Field Theory of Materials (CFTM2) .....	<u>6667</u>
Matlab Primer [Computational Methods Hub] .....	<u>6970</u>
Introduction to HPC .....	<u>6970</u>
Numerical Methods .....	<u>6970</u>
Group Programming Project .....	<u>7071</u>
Group Research Strategy Project (GRSP) .....	<u>7273</u>
<b>Appendix 2 Guidelines for the Conduct and Assessment of Research Projects</b>	<b><u>7576</u></b>

## Welcome to the College

Congratulations on joining Imperial College London, the only university in the UK to focus exclusively on science, medicine, engineering and business.

From Fleming's discovery of Penicillin to Gabor's invention of holography, Imperial has been changing the world for well over 100 years. You're now part of this prestigious community of discovery and we hope you will take this opportunity to make your own unique contribution.

We're committed to providing you with the very best academic resources to enrich your experience. We also provide a dedicated support network and a range of specialist support services to make sure you have access to the appropriate help, whether that's further training in an academic skill like note taking or simply having someone to talk to.

You'll have access to an innovative range of professional development courses within our Graduate School throughout your time here, as well as opportunities to meet students from across the College at academic and social events – see page 6 for more information.



We actively encourage you to seek out help when you need it and try to maintain a healthy work-life balance. Our choice of over 340 clubs, societies and projects is one of the largest of any UK university, making it easy to do something different with your downtime. You also have access to gym and swimming facilities across our campuses for an annual fee of £30.

As one of the best universities in the world, we are committed to inspiring the next generation of scientists, engineers, clinicians and business leaders by continuing to share the wonder of what we do through public engagement events. Postgraduate students, alongside our academics and undergraduate students, make a significant contribution to events such as our annual Imperial Festival and our term-time Imperial Fringe events – if you're interested in getting involved then there will be opportunities for you to do so.

## Our Principles

In 2012 the College and Imperial College Union agreed 'Our Principles' a series of commitments made between students and the College. The Principles are reviewed annually by the Quality Assurance and Enhancement Committee and changes recommended for Senate approval.

### **Imperial will provide through its staff:**

- A world class education embedded in a research environment
- Advice, guidance and support
- The opportunity for students to contribute to the evaluation and development of programmes and services

### **Imperial will provide students with:**

- Clear programme information and assessment criteria
- Clear and fair academic regulations, policies and procedures
- Details of full programme costs and financial support
- An appropriate and inclusive framework for study, learning and research

### **Imperial students should:**

- Take responsibility for managing their own learning
- Engage with the College to review and enhance provision
- Respect, and contribute to, the Imperial community

### **The Imperial College Students' Union will:**

- Support all students through the provision of independent academic and welfare assistance
- Encourage student participation in all aspects of the College
- Provide a range of clubs, societies, student-led projects and social activities throughout the year
- Represent the interests of students at local, national and international level

## Welcome from the Graduate School



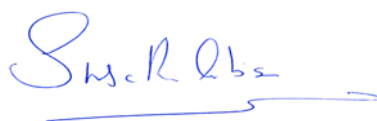
**Professor Sue Gibson,  
Director of the Graduate  
School**

The Graduate School has several roles but our main functions are to provide a broad, effective and innovative range of professional development workshops and to facilitate interdisciplinary interactions by providing opportunity for students to meet at academic and social events. Whether you wish to pursue a career in academia, industry or something else, professional skills development training will improve your personal impact and will help you to become a productive and successful researcher.

Professional development courses for Master's students are called "Masterclasses" and they cover a range of themes, for example, presentation skills, academic writing and leadership skills. All Masterclasses are free of charge to Imperial Master's students and I would encourage you to take as many as you can to supplement your academic training. The Graduate School works closely with the Graduate Students' Union (GSU) and is keen to respond to student needs so if there is an area of development training, or an activity that you would like us to offer, but which is not currently provided, please do get in touch ([graduate.school@imperial.ac.uk](mailto:graduate.school@imperial.ac.uk)).

The Graduate School also runs a number of exciting social events throughout the year which are an opportunity to broaden your knowledge as well as to meet other students and have fun. You should regularly check the Graduate School's website and e-Newsletters to keep up to date with all the events and development opportunities available to you.

Finally, I hope that you enjoy your studies here at Imperial, and I wish you well.



Sue Gibson



**Dr Janet De Wilde,  
Head of Postgraduate  
Professional Development**

I would like to welcome you to the Graduate School's programme of professional development for Master's students.

Our team of tutors come from a wide variety of experiences and we understand just how important it is to develop professional skills whilst undertaking postgraduate studies. Not only does our programme help you to progress in your academic studies, it can also be part of your preparation for your future career. We provide the opportunity for you to practice your presentation skills, academic writing skills and other key skills. It will also give you the chance to meet students from a variety of subject disciplines building your network.

We offer a range of interactive courses including face-to-face workshops, interactive webinars and online self-paced courses. I encourage you to explore and engage with the diverse range of opportunities on offer from the Graduate School and I wish you well in your studies.



## The Graduate School

You automatically become a member of the Graduate School when you register as a postgraduate student at Imperial.

The Graduate School has been set up to support all postgraduate students at the College through:

- Training and development courses
- Networking activities, social and academic events to encourage cross-disciplinary interactions
- Forums to represent the views of postgraduate students throughout the College

### 'Masterclass' professional skills courses

You can see the full range of free professional skills courses for postgraduate students on the Graduate School website:

 [www.imperial.ac.uk/study/pg/graduate-school/professional-skills/masters](http://www.imperial.ac.uk/study/pg/graduate-school/professional-skills/masters)

All courses can be booked online.



### Contact us



Level 3, Sherfield Building, South Kensington Campus



020 7594 1383



[graduate.school@imperial.ac.uk](mailto:graduate.school@imperial.ac.uk)



[www.imperial.ac.uk/graduate-school](http://www.imperial.ac.uk/graduate-school)

## Welcome from the Graduate Students' Union (GSU)



I am delighted to welcome you to Imperial College! Let me introduce you to the Graduate Students' Union (GSU). We are the representative body defending your interests as a post-graduate student in major decisions taken by the College. Beyond that, we work towards building a thriving post-graduate community that spans faculties and where students effectively communicate in an interdisciplinary way. Our committee is comprised by motivated post-graduate students like yourself, who have been appointed in university-wide elections and volunteer to make your experience at Imperial as fulfilling and enjoyable as possible.

So, what are we up to for this coming year 2018/19? We are going to focus on three major areas of action:

- Continue improving post-graduate well-being by increasing the quality of supervision and by creating strategies to tackle common mental health challenges in higher education.
- Develop the GSU to become central to the post-graduate community by improving the two-way flow of information, between the GSU and you.
- Organise exciting events around the topics of well-being, interdisciplinary research, and entrepreneurship.

As the GSU president, I would like to emphasise that Imperial College London is relying on its post-graduate students to maintain its position as a front-runner in world-class research and teaching. For us, the GSU, to be successful we need to receive as much of your input as possible. We want to work with you, for you!

Finally, I hope that you have a fantastic time here at Imperial and take advantage of the richness of opportunities that awaits you. If ever you have questions or ideas to share with us, please do not hesitate to get in touch with us and we are looking forward to seeing you at our events!

Ute Thiermann, GSU President 2018/19

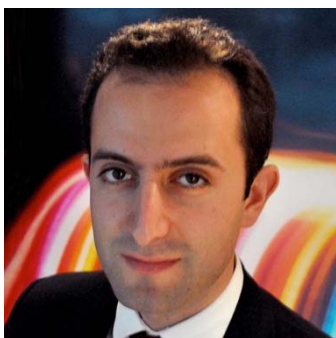
 [gsu.president@imperial.ac.uk](mailto:gsu.president@imperial.ac.uk)

 [www.imperialgsu.com](http://www.imperialgsu.com)



# 1. Introduction to the Department

## 1.1 Welcome from the CDT Director



The MSc in Theory and Simulation of Materials (TSM) runs under the auspices of the Centre for Doctoral Training (CDT) in TSM. The course is the brainchild of Prof. Adrian Sutton FRS, founding Director and member of the Strategic Advisory Team of the CDT, who had long foreseen the need for a mathematically rigorous and multidisciplinary training in the theory of materials and the methods used to simulate them. The course therefore spans many orders of magnitude in length- and time-scales: from the quantum-mechanical treatment of electrons, through phase-field models of microstructure, to finite element calculations for the continuum limit. It covers topics

traditionally confined to the territory of single disciplines: chemistry, physics, materials science and engineering. Whatever your own background, this course will expose you to subjects you have never encountered before. Graduates of this MSc will be more thoroughly equipped than ever before to tackle the complex, multiscale materials problems that arise in modern technologies from nuclear reactors to mobile phones.

Originally established in 2009 by a grant from the Engineering and Physical Sciences Research Council (EPSRC), in 2013 the TSM-CDT was awarded funding to train a further five cohorts of students. As part of the proposal for continued funding, this MSc has been reviewed and revised, with the following aims in mind:

- i. to maintain the ethos of continuous innovation;
- ii. to increase the engagement of our external partners in the delivery of the training;
- iii. to promote the development of students' self-reliance and independence in learning, in preparation for research;
- iv. to provide more opportunities for peer learning, e.g. through group projects;
- v. to introduce a more comprehensive training in computational methods;
- vi. to facilitate the involvement of a wider range of academic staff in the delivery; and
- vii. to create more time for the research project and particularly for the literature review.

Our goal is to make the TSM-CDT an enriching, challenging and supportive environment that is conducive to learning and scholarship. We hope, therefore, that all of you will engage constructively with us as partners to help us identify problems, devise solutions and ensure that we continue to deliver a cutting-edge training experience that provides the best possible preparation for research in TSM.

Interest in the TSM-CDT has been registered by over 80 academics at Imperial from the nine Departments of Aeronautics, Chemical Engineering, Chemistry, Civil & Environmental Engineering, Earth Science & Engineering, Materials, Mathematics, Mechanical Engineering and Physics across the Faculties of Engineering and Natural Sciences as well as those from other academic institutions and researchers who work for our industry partners. This reflects the strength and breadth of expertise in the College on TSM and the wide range of research topics that will be available to you.

The TSM-CDT also benefits from the Thomas Young Centre ([www.thomasyoungcentre.org](http://www.thomasyoungcentre.org)), the London Centre for TSM. The TYC is a federation of research groups involved in TSM at Imperial, King's College, UCL and Queen Mary's. It provides an outstanding program of seminars, workshops, conferences, distinguished visitors, and short courses by experts from around the world, all of which are available to everyone in the TSM-CDT. You are strongly encouraged to participate in the events organised by the TYC to further enrich your educational and social experience.

We hope our course will prove attractive to mathematically oriented students of physical sciences and engineering around the world. For more information about the CDT visit [www.tsmcdt.org](http://www.tsmcdt.org)

## 1.2 About This Handbook

The purpose of this handbook is to provide current students and staff with a detailed description of the MSc in Theory and Simulation of Materials (TSM) course run by the EPSRC Centre for Doctoral Training (CDT) in TSM, including assessment and feedback mechanisms (where appropriate).

This edition of the handbook applies to the academic year 2018–19. An electronic copy of this handbook will be provided to every student at the start of the academic year and any significant changes to its content will be communicated to them. A copy of the current handbook will be made available online at the course Blackboard site and on the CDT web site [www.tsmcdt.org](http://www.tsmcdt.org).

The MSc course usually has a relatively small number of students (in comparison to many undergraduate courses) and they have extensive access to the academic and support staff of the TSM-CDT. Students therefore should not hesitate to approach the MSc Director or any member of staff for advice or assistance.

**This handbook describes the framework of the course and its assessment but the MSc Director and/or Course Committee may make changes to detailed procedures if the circumstances indicate that this is desirable. Similarly, the Board of Examiners has absolute discretion to modify the criteria described in this handbook, although in practice this would only occur in exceptional circumstances. Students will be notified of any changes prior to their introduction.**

## 1.3 Aims and Objectives of the MSc in Theory and Simulation of Materials

The formal aim of the MSc in Theory and Simulation of Materials is “to train students in the core concepts and methods of theoretical and computational materials physics necessary for doctoral study in the field or for a technical career outside academia.”

This aim is fulfilled via the following formal objectives. The MSc in TSM will:

- attract well-qualified Bachelor level students and provide an intellectually challenging degree programme;
- provide high quality advanced education in materials theory and simulation beyond Bachelor level within an environment with considerable teaching and research experience in the field;
- give students the experience of undertaking a major, individual project and reporting the results in a full scientific report and presentation;
- give students training in appropriate research methods, including comprehensive training in computational methods;
- develop students’ skills of communication, both written and oral, peer learning and teamwork;
- equip students for further academic study at doctoral level in materials physics and subjects where this is an important enabling science, such as aerospace, automotive transport, renewable energy, health-care and construction.

The key elements of the course that support these objectives are:

- about 100 lectures and 50 tutorials, rapid feedback sessions and computational classes in core and optional subjects in the first two terms, assessed by written and oral examinations, as well as assessed exercises and problem-solving;
- courses offered by the Graduate School, which are optional during the MSc;
- a four-month individual research project, assessed by a literature review, an oral presentation and a written report.

## 1.4 The Centre for Doctoral Training on Theory and Simulation of Materials

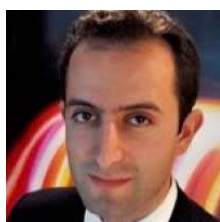
The Engineering and Physical Sciences Research Council (EPSRC) established the TSM-CDT in 2009, with the intention of training a cadre of physical scientists and engineers with advanced skills in TSM, an area in which there is recognised to be a national and international shortage of trained people. Funding for a further five cohorts was awarded in 2013. The CDT draws upon the expertise of the Departments of Physics, Materials, Chemistry, Mechanical Engineering, Aeronautics, Chemical Engineering, Mathematics, Earth Science & Engineering and Civil & Environmental Engineering at Imperial College plus academic staff at UCL and King's College London via the Thomas Young Centre. The CDT works closely with the other Centres based in the College and with other academic departments working in TSM.

For administrative purposes, including quality assurance and oversight, students are registered for the MSc degree in the Department of Physics where they have full access to departmental support structures in addition to those provided by the CDT. These include Dr Andrew Williamson and Ms Loli Sanchez Rey in the postgraduate administration office, and Dr William Proud the Director of Postgraduate Studies. The Department of Physics taught Masters webpages may be found here: <https://www.imperial.ac.uk/natural-sciences/departments/physics/students/current-students/taught-postgraduates/>

## 1.5 Academic and Administrative staff

A full list of academic staff involved in the CDT may be found on our website:


<http://www.imperial.ac.uk/theory-and-simulation-of-materials/people/staff/> Most contribute to the MSc course either directly or indirectly. The following table lists those with administrative responsibility.



 Dr Arash Mostofi

CDT Director

 332 Bessemer

 48154

 a.mostofi@imperial.ac.uk



 Dr Johannes Lischner

CDT Assistant Director &  
Cohort Mentor (2018 entry)

 342 Bessemer


 49949

 j.lischner@imperial.ac.uk



 Prof Peter Haynes

Strategic Advisory Team

 201B Royal School of Mines

 45158

 p.haynes@imperial.ac.uk



 Prof Adrian Sutton


Strategic Advisory Team

 a.sutton@imperial.ac.uk



 Prof Dimitri Vvedensky

Admissions Tutor

 813 Blackett

 47605

 d.vvedensky@imperial.ac.uk



 Dr Andrew Horsfield


Cohort Mentor (2015 entry)




 331 Bessemer

 46753

 a.horsfield@imperial.ac.uk






 Dr Kim Jelfs  
Cohort Mentor (2016 entry)


 134C Chemistry  
 43438  
 k.jelfs@imperial.ac.uk






 Prof Daniele Dini  
Cohort Mentor (2017 entry)


 669, City and Guilds Building  
 47242  
 d.dini@imperial.ac.uk






 Dr Simon Foster  
Outreach Officer


 313 Blackett  
 42945  
 simon.foster1@imperial.ac.uk



 Miss Miranda Smith  
CDT Senior Administrator

 EPSRC CDT Suite  
 40709  
 Miranda.smith@imperial.ac.uk



 Miss Naho Ollason  
CDT Administrator

 EPSRC CDT Suite  
 45609  
 n.ollason@imperial.ac.uk

The Director and other staff will provide information to students through one of several channels, depending upon the nature of the information (e.g. confidential or not):

- e-mail;
- via the MSc course Blackboard site;
- on the notice boards in the CDT Suite;
- letter delivered by internal mail;
- letter to your home address;
- personal communication before/after lectures or during classes.

**In particular, students are expected to check their College email account at least once a day during term and while undertaking the research project.**

## 1.6 Student Representation

There is one elected student representative from each cohort who serves on the CDT Operations Board, usually for a fixed term of one year. The representative from the cohort currently undertaking the MSc will also serve as the student representative on the MSc Course Committee in the Department of Physics, and students are encouraged to raise general or specific matters through this channel as well.

Any concerns of a more urgent or personal nature should be discussed with the appropriate Cohort Mentor or the CDT Director.

The College has an online mechanism to evaluate each and every course called PG SOLE: Postgraduate Student Online Evaluation. Each student is asked to complete this survey about the course towards the end of Terms 1 and 2. The results are discussed at the MSc Course Committee with a view to addressing any concerns in the future.

## 1.7 English Language Requirement

If you are not a native English speaker you must meet the College's English language requirements.

See the Admissions website for details:

 [www.imperial.ac.uk/study/pg/apply/requirements/english](http://www.imperial.ac.uk/study/pg/apply/requirements/english)

For information on English language support available while you're here, see section 9.8.

## 1.8 Attendance and Absence

The CDT is responsible for monitoring student attendance. If you are unable to attend a lecture or event please notify the lecturer in advance. Students hand in their solutions to problem sets each week, this enables staff to monitor attendance.

You must inform your Cohort Mentor or the CDT Senior Administrator if you are absent from the College for more than three days during term. If the absence is due to illness you must produce a medical certificate after seven days. If you miss an examination through illness you must contact the CDT Senior Administrator on the day and provide a medical certificate within five working days.

The Registry will be informed of all student non-attendances as the College is obliged to report the non-attendance of students on Tier 4 visas to the Home Office.

**If coursework is affected students must complete a (minor) mitigating circumstances form as soon as possible.**

**If a student misses an examination because they are ill it is essential that they obtain a medical certificate and complete a (major) mitigating circumstances form as soon as possible.**

Further information on the College's policy and procedures for mitigating circumstances can be found at <http://www.imperial.ac.uk/natural-sciences/departments/physics/students/current-students/student-welfare/mitigating-circumstances/>

Note that absences due to work commitments are not admissible as mitigating circumstances, and in general due to the demands of this course, part-time employment is strongly discouraged.

## 1.9 Key dates 2018-19

### Term dates

Autumn term:	29 September - 14 December 2018
Spring term:	5 January - 22 March 2019
Summer term:	27 April - 28 June 2019



## Closure dates

Christmas/New year:	22 December 2018 - 1 January 2019 (College reopens on 2 January 2018)
Easter:	18 April - 23 April 2019 (College reopens on 24 April 2019)
Early May bank holiday:	6 May 2019
Spring bank holiday:	27 May 2019
Summer bank holiday:	26 August 2019

## Key Programme dates

The course is described in more detail in section 2. The following outline is approximate: lectures and classes may need to be rescheduled due to staff absence etc.

### TERM 1

Week 1	Introduction to the MSc Provost's welcome address Group project (cohort challenge) Safety briefing and reception in Physics TSM welcome lunch
Week 2	Election of Student Representative for the new cohort
Weeks 2–5	Lectures and classes for core courses
Week 6	Reading week*
Weeks 7–10	Lectures and classes for core courses
Week 11	Revision week*

### TERM 2

Week 1	Written Examinations – all courses delivered in Term 1 Group projects commence
Weeks 2–5	Lectures and classes for core and advanced courses
Week 6	Reading week*
Weeks 7–10	Lectures and classes for core and advanced courses
Week 11	Oral Examinations – courses delivered in Term 2

### TERM 3 and SUMMER VACATION

April	Literature review starts
May	Start of research project Presentations/interviews for group projects E-MRS Spring Meeting**
June/July	Industry site visit
Late August	Project presentations
Early September	Project report submission
Late September	Examiners' Meeting
Day of Examiners' Meeting	Informal Notice of Results (usually around 4pm)

\* We endeavour to keep Reading and Revision weeks free from timetabled commitments, but this is usually not possible in practice and students should expect there to be some timetabled classes, though much fewer than in other weeks during term.

\*\* This is just one suggestion of a possible cohort conference trip. The actual conference attended will be decided through discussion with the Cohort Mentor and may occur earlier or later in the year.

## 2. Programme Information

### 2.1 Administration

The MSc in TSM is administered day-to-day by the CDT Administrators, Miss Miranda Smith and Miss Naho Ollason, working closely with the CDT Director, academic and administrative staff in the Departments participating in the CDT. The CDT Operations Board and the MSc Course Committee of the Department of Physics oversee the course and make changes to the course content and organisation as appropriate. The CDT Operations Board meets weekly through term time and at least monthly out of term time. The MSc Course Committee of the Department of Physics meets once a term. The members of the CDT Operations Board are:

Dr Arash Mostofi (CDT Director and Chair)  
Dr Johannes Lischner (Assistant CDT Director)  
Student Representatives  
Cohort Mentors  
Dr Simon Foster (Outreach Officer)  
Miss Miranda Smith (Senior Administrator)  
Miss Naho Ollason (Administrator)

The members of the MSc Course Committee of the Department of Physics from the CDT are:

Dr Arash Mostofi  
Student Representative of the MSc cohort

### 2.2 Timetables and the Working Day

The MSc term dates are the same as those for undergraduate courses at Imperial College except for the summer term (details available in section 1.9). Lecture courses run during the first two terms. Examinations and major assessments are held at the start and end of the second term and start of the third term. Work on the literature review starts after Easter as an introduction to the research project that follows. The project continues through the rest of the summer term and into the undergraduate summer vacation, finishing in mid-September. Timetables for each term are prepared in time for the start of term and are distributed to all students. These contain details of all lectures, rapid feedback (problem) classes, computational classes, examinations, presentations and deadlines. If an examination or major assessment is scheduled to clash with a religious obligation, please consult the CDT Director. The College's policy is online: <http://www.imperial.ac.uk/student-records-and-data/for-current-students/undergraduate-and-taught-postgraduate/exams-assessments-and-regulations/exams-and-religious-obligations/>

The College standard working day is used, with 50-minute lectures *commencing on the hour*, starting at 9am each day. In Term 1, there are 16 timetabled hours a week on average during the eight main teaching weeks (weeks 2–5 and 7–10). During week 1 students undertake a “cohort challenge”, week 6 is a reading week and week 11 is intended for revision. In Term 2, there are approximately 10 timetabled hours during the eight main teaching weeks. Written examinations are held in week 1, week 6 is a reading week and week 11 is intended for revision and oral examinations. An attempt is made to keep Wednesday afternoons free for other activities. Lectures and rapid feedback classes (i.e. problem classes) are usually held in the EPSRC CDT Suite. Some lectures may be held elsewhere, e.g., in the Department of Physics.

## 2.3 The Curriculum

### 2.3.1 Overview

There are two main elements to the MSc course, with the following contributions to the final mark:

- *Taught course element.* This is assessed by written and oral examinations, problem sets, computational classes and other exercises. It counts for 60% of the overall mark (defined in detail in section 3).
- *Research project element.* This is assessed by literature review, an oral presentation and a written report at the end of the project, and counts for 40% of the overall course mark.

To be awarded an MSc, students are required to satisfy the requirements explained in section 3.3. This section also explains the requirements for the award of a “Merit” and “Distinction”.

An illustration of the structure of the MSc programme is shown below:

Week	1	2	3	4	5	6	7	8	9	10	11
Term 1	Cohort challenge	<b>MTM 1 – core</b> <b>EQM 1 – core</b> <b>ESM 1 – core</b> <b>CMM – core</b>				Reading week	<b>MTM 2 – core</b> <b>TM 1 – core</b> <b>CFTM 1 – core</b> <b>CMM – core</b>				Revision
Term 2	Written exams	<b>MSM 1 – core</b> <b>EQM 2 – advanced</b> <b>TM 2 – advanced</b> <b>ESM 2 – advanced</b> <b>CFTM 2 – advanced</b> <b>CMM – core</b>				Reading week	<b>MSM 2 – core</b> <b>EQM 2 – advanced</b> <b>TM 2 – advanced</b> <b>ESM 2 – advanced</b> <b>CFTM 2 – advanced</b> <b>CMM – core</b>				Oral exams
		<b>GRSP – core</b>									
Term 3	Literature review			Research project							
Summer	Research project										

### 2.3.2 Taught Courses

All students must take the compulsory parts of the *core courses*. These six subjects are:

- Mathematics for Theory of Materials (MTM);
- Equilibrium in Materials (EQM);
- Transformations of Materials (TM);
- Electronic Structure of Materials (ESM);
- Classical Field Theory of Materials (CFTM);
- Methods for Simulating Materials (MSM).

During Term 1 all courses are compulsory, and comprise six *parts*:

- Mathematics for Theory of Materials: Parts 1 and 2 (MTM1 and MTM2);
- Equilibrium in Materials: Part 1 (EQM1);

- Transformations of Materials: Part 1 (TM1);
- Electronic Structure of Materials: Part 1 (ESM1);
- Classical Field Theory of Materials: Part 1 (CFTM1).

Each part consists of 16 lectures with four rapid feedback classes, with the exception of MTM, which in total (ie, Parts 1 & 2) consists of 24 lectures and 7 rapid feedback classes.

During Term 2 all students take the compulsory sixth subject:

- Methods for Simulating Materials (MSM1 and MSM2).

This course is delivered through 16 lectures and 16 hours of hands-on computational classes and feedback sessions.

In addition, during Term 2, students select two *advanced courses*, which comprise the second parts of four subjects:

- Equilibrium in Materials: Part 2 (EQM2);
- Transformations of Materials: Part 2 (TM2);
- Electronic Structure of Materials: Part 2 (ESM2);
- Classical Field Theory of Materials: Part 2 (CFTM2).

These courses will be delivered through directed reading, and about eight discussion classes.

Students also take the Computational Methods for Materials (CMM) course during Terms 1 and 2, and the Group Research Strategy Project during Term 2.

### 2.3.3 Rapid Feedback Classes

Rapid feedback classes are held approximately every week for each of the standard lecture courses. They may consist of problems that are worked through during the class, discussions or further explanation of the material. Students are encouraged to liaise with the lecturer to help set the agenda for these classes.

### 2.3.4 Computational Methods

Training in computational methods is given during Terms 1 and 2 via the Computational Methods for Materials (CMM) course, consisting of a general introduction to tools for programming, Python and C/C++, followed by training in numerical methods and a group project.

### 2.3.5 Industrial Engagement

An appreciation of the role of materials in industry, and TSM in particular, is an important part of the training provided by the CDT. To this end there will be a number of “Materials Challenge” lectures delivered by external partners during the year and an industry site visit. All students are expected to attend all of these events.

### 2.3.6 Literature Review

The literature review begins after the conclusion of the oral exams at the end of Term 2 as a prelude to the research project (on the same topic). This must be submitted electronically as a report in PDF format (3,000 words maximum) by **5pm on 10 May 2019** to the CDT Senior Administrator. The literature review accounts for 10% of the total marks available in the MSc.

### 2.3.7 Research Project

The research element of the project starts in the summer term. Each student is required to give an oral presentation about the project at the MSc conference on **30 August 2019**. The project report must be submitted electronically in PDF format (5,000 words maximum, excluding appendices) by **5pm on 6 September 2019** to the CDT Senior Administrator.

The research project may be carried out at Imperial College or at a partner institution of the CDT or another academic institution, where appropriate arrangements exist. All students have a project supervisor at Imperial College and any student carrying out the project elsewhere must also have an Imperial College supervisor.

The research project (excluding the literature review) accounts for 30% of the total marks available in the MSc. One fifth of the marks for the project are assigned to the oral presentation and four fifths to the written report. The report is marked independently by two members of staff.

Further details about the research project and its assessment are provided in Appendix 2.

### 2.3.8 Blackboard

Some of the material for the lecture courses may be delivered using the Blackboard Learning System, a Virtual Learning Environment (VLE), which can be used to access material, such as lecture notes and problem sheets posted by the course lecturer. Past exam papers may also be found there. Different lecture courses use Blackboard to differing degrees and you will be advised by each lecturer about the material they have made available. You will need to register with the course before you can access the material. In most cases this will be done upon your arrival but please contact [andrew.williamson@imperial.ac.uk](mailto:andrew.williamson@imperial.ac.uk) if you wish to gain access for a particular course.

Log on to Blackboard at [bb.imperial.ac.uk](http://bb.imperial.ac.uk).

### 2.3.9 Outreach

Our Outreach Officer, Dr Simon Foster, works with CDT students to help them develop and practise a range of communication skills for various audiences. Besides their presentation abilities, students also hone a capacity to structure and present complex information, which will aid them throughout their academic careers and beyond. During the MSc, participation in these activities is optional but nevertheless encouraged. If you would like to get involved then email [simon.foster1@imperial.ac.uk](mailto:simon.foster1@imperial.ac.uk).

## 2.4 Imperial Mobile app

Don't forget to download the free Imperial Mobile app for access to College information and services, including your programme timetable, College emails and a library catalogue search tool.

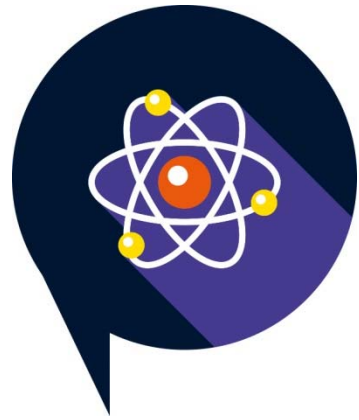
 [www.imperial.ac.uk/imperialmobile](http://www.imperial.ac.uk/imperialmobile)



## 2.5 Imperial Success Guide

The Imperial Success Guide is an online resource with advice and tips on the transition to Master's level study. More than just a study guide, it is packed with advice created especially for Imperial Master's students, including information on support, health and well-being and ideas to help you make the most of London.

 [www.imperial.ac.uk/success-guide](http://www.imperial.ac.uk/success-guide)



## 3. Assessment

### 3.1 Overview

This section details the assessment procedures for each element of the MSc course. The distribution of marks between the different elements of assessed work is summarised below.

Activity	Total marks	Written Exam	Oral Exam or Presentation	Assessed Coursework	Written Report
Compulsory core (MTM1&2, EQM1, TM1, ESM1, CFTM1, MSM1&2)	320 (35.6%)	192 (21.3%)	24 (2.7%)	104 (11.6%)	
Advanced core (two of EQM2, TM2, ESM2, CFTM2)	80 (8.9%)		40 (4.4%)	40 (4.4%)	
Computational methods	60 (6.7%)			60 (6.7%)	
Group project	80 (8.9%)		26.7 (3.0%)		53.3 (5.9%)
Literature review	90 (10%)				90 (10%)
Research project	270 (30%)		54 (6.0%)		216 (24%)
Total	900 (100%)	192 (21.3%)	144.7 (16.1%)	204 (22.7%)	359.3 (39.9%)

For each of the compulsory core courses MTM1&2, EQM1, TM1, ESM1 and CFTM1, 20% of the marks come from assessed coursework and 80% from the written examinations in January. For MSM the whole mark comes from assessed coursework, including an oral presentation.

The percentage (which has been rounded to the nearest 0.1%) under each heading indicates the weighting used in calculating the overall course mark. These notes are intended to assist students, by showing the basis and criteria on which marks are awarded, and staff in standardising the assessment procedures as applied from student to student, and from year to year.

*The Examiners nevertheless reserve the right to make adjustments to the procedures given in this section in exceptional circumstances.*

Formal feedback to the students in each activity is by way of a letter grade indicating the percentage band of their attainment. The definition of the letter grades is given in §3.6 below.

All of the marks are reviewed at a meeting of a sub-board of the Board of Examiners, usually comprised of the CDT Director, Assistant Director and Cohort Mentor. This sub-board is informed by staff involved in the MSc course, who may suggest that the examiners take into account any special factors. This board also acts as the Mitigation Advisory Panel that takes into account any mitigating circumstances that have been submitted by students (see §4.1 below). The marks are then forwarded to the External Examiner for information. The Board of Examiners, comprised of the External Examiner and all staff involved in the delivery of the course, meets in late September or early October to review all the marks and make final recommendations to the College. It is traditional to send a

copy of the project reports to the External Examiner in advance of this meeting, to provide additional information that might assist the decision process. The marks presented before the Board of Examiners for the MSc in TSM is anonymous (i.e., student names do not appear with the marks that are being considered).

## 3.2 In Detail

### 3.2.1 The Marks Available

There are **TWO** assessed elements of the MSc:

- (1) the taught element, consisting of SEVEN components (combinations of courses):
  - (a) Mathematics for Theory of Materials (MTM1 and MTM2)
  - (b) Equilibrium in Materials (EQM1) and Transformations of Materials (TM1)
  - (c) Electronic Structure of Materials (ESM1) and Classical Field Theory of Materials (CFTM1)
  - (d) Methods of Simulating Materials (MSM1 and MSM2)
  - (e) Advanced parts of the core courses, TWO chosen from the following FOUR options:
    - o Equilibrium in Materials (EQM2)
    - o Transformations of Materials (TM2)
    - o Electronic Structure of Materials (ESM2)
    - o Classical Field Theory of Materials (CFTM2)
  - (f) Group Research Strategy Project (GRSP)
  - (g) Computational Methods for Materials (CMM)
  
- (2) the research element, consisting of TWO components:
  - (h) Literature Review
  - (i) Research Project

The marks (credits) available for each component are as follows:

- (a) MTM1 and MTM2: 80 marks (8 ECTS) in total – 16 marks for assessed problems, 64 marks from the written examination
- (b) EQM1 and TM1: 80 (8 ECTS) in total – 16 marks for assessed problems and 64 marks from the written examination
- (c) ESM1 and CFTM1: 80 (8 ECTS) in total – 16 marks for assessed problems and 64 marks from the written examination
- (d) MSM1 and MSM2: 80 marks (8 ECTS) in total – 56 marks for assessed exercises and 24 marks from an oral presentation
- (e) Advanced parts (two chosen from EQM2, TM2, ESM2, CFTM2): 80 marks (8 ECTS) in total – 40 marks for assessed coursework and 40 marks from the oral examinations
- (f) Group project (GRSP): 80 marks (8 ECTS) in total – 53.3 marks for a written proposal, 26.7 marks for a presentation and panel interview. A proportion of these marks is awarded by peer-to-peer allocation (see GRSP outline for more details)
- (g) CMM: 60 marks (6 ECTS) in total – for assessed coursework. A proportion of these marks is awarded by peer-to-peer allocation (see CMM course outline for more details)
- (h) Literature review: 90 marks (9 ECTS) in total – assessed by a written report of no more than 3,000 words, excluding appendices
- (i) Research project: 270 marks (27 ECTS) in total – 216 marks for the written report and 54 marks for the oral presentation<sup>1</sup>

For the elements as a whole:

- (1) Taught element (a)–(g): 540 marks (54 ECTS) in total

---

<sup>1</sup> Further information about reporting progress during the research project, the assessment criteria, the structure of the report, and marking of the report are provided in Appendix 2.



(2) Research element (h)–(i): 360 marks (36 ECTS) in total

**Totals for the course: 900 marks (90 ECTS)**

### 3.2.2 Schedule of Examinations

Written examinations for the six compulsory parts of the core courses taught in Term 1 will take place in the first week of Term 2. Written examinations normally last 2 hours. Rubrics will be circulated to students during Term 1.

Oral examinations for the advanced parts of core courses taught in Term 2 will normally take place in the last week of Term 2. The oral presentation/examination for the group projects will normally be held during Term 3.

### 3.2.3 Marking of Problem Sets

For many courses assessed problems will be set weekly while lecture courses are running. They will be graded either by the lecturer or by teaching assistants. Students will receive feedback including a letter grade for each problem set, according to the following criteria:

$\alpha$  (alpha): mostly correct with only a little wrong

$\beta$  (beta): slightly more correct than wrong

$\gamma$  (gamma): some correct elements but mostly wrong

$\delta$  (delta): almost entirely wrong

$\emptyset$  (null): did not hand in the problems on time, or entirely wrong

Each assessed problem set should take you around 2 hours to complete. If it is taking you significantly longer please speak to the lecturer or your cohort mentor.

Deadlines for handing in assessed coursework are indicated on the course timetable. Unless the course lecturer makes alternative arrangements or another time is specified, work should be handed in to the CDT Administration Office by 5pm on the day of the deadline. Late submissions will be handled under the College's Late Submission Policy (see section 8.4). In summary:

Late work will be capped at the pass mark where it is up to one calendar day (24 hours) late. A mark of zero will be awarded for work that is more than one calendar day (24 hours) late. Work submitted up to one day after the deadline should be marked and feedback given. Work submitted more than one day late may receive feedback at the discretion of the Operations Board and/or course lecturer.

Acceptable reasons for failing to hand in work on time are the usual ones such as illnesses or significant personal problems. If you know you are going to miss a deadline you **must complete a minor mitigating circumstances form** available from the CDT Administrators, which will be considered by the Operations Board. You should also inform the lecturer concerned as a matter of courtesy.

You are strongly encouraged to collaborate with other students in your cohort by discussing your approaches and solutions to the problems with each other. However, when you write down your solutions you must do so by yourself. Copying another student's work and presenting it as your own constitutes cheating and is subject to the College's disciplinary procedures.

The College statement regarding plagiarism follows. Early in the academic year you will attend a compulsory workshop on research ethics that covers plagiarism to ensure that you understand what it involves and how to avoid it. This will be followed by an opportunity to take the College's online course and test on plagiarism that is compulsory for all Master's students.

### 3.2.4 Plagiarism

Plagiarism is the presentation of another person's thoughts, words, images or diagrams as though they were your own. Another form of plagiarism is self-plagiarism, which involves using your own prior work without acknowledging its reuse.

Plagiarism is considered a cheating offence and must be avoided, with particular care on coursework, essays, reports and projects written in your own time and also in open and closed book written examinations.

Where plagiarism is detected in group work, members of that group may be deemed to have collective responsibility for the integrity of work submitted by that group and may be liable for any penalty imposed, proportionate to their contribution.

For further information, please refer to the [Academic Misconduct Policy and Procedures](#) section 8.6 of this handbook.

#### Imperial College Statement regarding Plagiarism

Students should be aware of the need to give proper credit for the work of others when writing papers, reports, theses, etc. This is particularly important when the work is in collaboration with other persons. The College's advice on [Academic Integrity](#) (linked from this webpage: <https://www.imperial.ac.uk/about/governance/academic-governance/academic-policy/exams-and-assessment/>) contains a section on plagiarism, which is reproduced here:

*You are reminded that all work submitted as part of the requirements for any examination and assessment (including coursework) must be expressed in your own words and incorporate your own ideas and judgements.*

*Plagiarism, which is the presentation of another person's thoughts, words or images and diagrams as though they were your own and which is a form of **cheating**, must be avoided, with particular care in coursework, essays, reports and projects written in your own time and also in open and closed book written examinations. You are encouraged to read and criticise the work of others as much as possible, and you are expected to incorporate this into your thinking and in your coursework and assessments. But you must be sure to **acknowledge and identify your sources**.*

*Direct quotations from the published or unpublished work of others, whether from the internet or from any other source, must always be clearly identified as such by the use of quotation marks, whether in coursework or in an open or closed book examination. A full reference to their source must be provided in the proper form. Remember that a series of short quotations from several different sources, if not clearly identified as such, constitutes plagiarism just as much as a single unacknowledged long quotation from a single source. Equally, if you summarise another person's ideas or judgements, figures, diagrams or software, you must refer to that person in your text, and include the work referred to in your bibliography. Departments are able to give advice about the appropriate use and correct acknowledgement of other sources in your own work.*

*Where plagiarism is detected this is most usually in project work or coursework i.e. work that is submitted in the candidate's own time but plagiarism can also occur in closed book written examinations. Such situations can arise where candidates have been able to learn text by heart [by rote] and simply reproduce what they have learnt without attribution. Where the examination is based on technical knowledge this may be acceptable and not regarded as plagiarism. In other subjects where candidates are asked to write essays the examiners may regard text reproduced without reference or critical analysis as plagiarism. Boards of Examiners are encouraged to clarify where appropriate in examination rubrics how sources should be acknowledged in those examinations.*

*The direct and unacknowledged repetition of your own work which has already been submitted for assessment can constitute **self-plagiarism**.*

*Where group work is submitted, this should be presented and referenced, with individual contributions recorded, in the convention appropriate to your discipline. You should therefore consult your personal or senior tutor or course director if you are in any doubt about what is permissible.*

*You should be aware that you have a collective professional responsibility as a group for the integrity of all of the work submitted for assessment by that group. If you become aware that a member or members of the group may have plagiarised part of the group's submission you have an obligation to report your suspicions to your personal or senior tutor or the course director.*

*The use of the work of another student, past or present, also constitutes plagiarism. Where work is used without the consent of that student, this will normally be regarded as a major offence of plagiarism. Giving your work to another student to use (other than in a group assessment) may also constitute an offence.*

*The College may submit your work to an external plagiarism detection service, and by registering with the College you are automatically giving your consent for any of your work to be submitted to such a service.*

*The College will investigate all instances where an examination or assessment offence is reported and apply appropriate penalties to students who are found guilty. These penalties include a mark of zero for the assessment in which the examination offence occurred or a mark of zero for **all** the assessments in that year or exclusion from all future examinations of the University (i.e. expulsion from the university).*

### 3.2.5 Use of Materials for Teaching

It is anticipated that all materials involved in the delivery of the course work will be made available to students electronically. Such materials may include lecture notes, problem sets and solutions, computational exercises and solutions, and recordings of lectures and problem classes etc. All this material is copyright, and students may not use it for any purpose other than their own private study, and they may not distribute it to anyone else in any medium. The penalties for infringing these rules are severe and they may include expulsion from Imperial College and prosecution under copyright law.

### 3.2.6 Use of Calculators in Written Examinations

The College Board of Graduate Studies has determined that only College-owned approved non-programmable calculators can be used in the written examinations. The Physics Department has approved and can provide calculators, which use algebraic logic. Appropriate arrangements will be made for students wishing to use reverse Polish notation (RPN) calculators. However, in all cases, only College-owned calculators may be used in the written examinations and therefore students are advised to either purchase an appropriate calculator or practise on a College-owned calculator before the written examinations.

### 3.2.7 Written Reports

Here are some general comments which are applicable to all MSc reports. All reports should be word processed. Margins should not be less than 20mm. Number all pages. Do not use fonts smaller than 11pt for the main text. Make sure diagrams, figures and graphs are clearly laid out with clear labels and captions.

**DEADLINES: The Board of Assessors reserves the right not to mark reports submitted late. Computer difficulties will not be accepted as excuses for late submission. Any extenuating circumstances (e.g. illness) should be discussed with the Director or Cohort Mentor immediately.**

### 3.2.8 Written Examinations

Draft examination papers are prepared by the lecturer, moderated by a second member of staff and sent in advance to the External Examiner who reviews them and may suggest changes. After discussion with the course lecturers, these changes are usually incorporated into the final papers.

Each examination question is normally marked out of 25 by the course lecturer; each question is then check marked by a second marker. The total mark for each paper is converted to a percentage, the corresponding letter grade being fed back to the student.

Past examination papers will be made available on Blackboard.

Students who are candidates for examinations are asked to note that all examinations are conducted in accordance with the College's Academic Regulations, the Regulations for Programmes of Study and the Examination Regulations.

Instructions for exam candidates can be found here:



<http://www.imperial.ac.uk/media/imperial-college/administration-and-support-services/registry/academic-governance/public/academic-policy/exam-arrangements-and-re-sits/Instructions-to-candidates-for-examinations.pdf>

### 3.2.9 Oral (viva voce) Examinations for Advanced Options

Oral examinations for the Advanced Option courses (EQM2, TM2, ESM2, and CFTM2) take place at the end of Term 2. They are designed to test your depth of knowledge in the subject. For each course, around one week in advance of your oral examination, you will be provided with a list of three topics. You choose one out of the three topics to be the focus of the questions in the oral examination. The examination will be conducted by the course lecturer; an independent member of staff will act as an observer and moderator, who will ensure a similar standard is set across all of the Advanced Option courses. No formal presentation is required- the format will be one in which the lecturer will ask questions on the chosen topic for the duration of the viva, which will be 15 minutes. If helpful or appropriate students may use the whiteboard or write things down on paper during the discussion. The oral examination is marked out of 100 by the lecturer and independent observer.

### 3.2.10 Literature Review and Research Project

The literature review is assessed by a written report and marked by the principal supervisor.

The research project is assessed via oral presentation and a written report. The final mark for the project is the weighted average of the oral presentation and the written report (weighting 1:4). The project report is marked by two independent assessors, informed by a report from the supervisor about the student's performance and any external factors that should be taken into account. In the event of significant disagreement between the marks awarded by the two markers, the markers will confer to arrive at a consensus mark. In the unlikely event that a consensus cannot be reached, the CDT Director and/or External Examiner will determine the final mark.

Guidelines for the conduct and assessment of literature reviews and research projects for the MSc in TSM may be found in Appendix 2.

### 3.2.11 Transferable Skills

Training in professional or transferable skills is embedded within the MSc in TSM course, e.g.:

- Writing skills: written work is a major part of the continuously assessed coursework. Written reports account for more marks than any other form of assessment, notably the literature review and report on the research project.
- Presentation skills: short talks contribute to the assessment of one of the group projects and the research project. Participating in outreach activities coordinated by Simon Foster is an excellent way of developing these skills.
- Research ethics: a one day course on research ethics covering topics such as plagiarism, scientific misconduct, whistleblowing and open access publishing will be given in Term 1 by Marianne Talbot, Director of Studies in Philosophy at the University of Oxford.
- Interview skills: several components of the course, including the advanced core parts, may be assessed by interview (oral examination).

- Computing and programming skills: the course will ensure that you become proficient in using a UNIX-based environment and programming in Python and/or C/C++, particularly through the computational methods classes.
- Networking and collaboration: the cohort-based approach to the course, together with the events organised by the Thomas Young Centre, provide excellent opportunities for networking and to develop skills in collaboration.

In addition the Graduate School offers a range of courses and these will be publicised during the year. Details can be found at

<https://www.imperial.ac.uk/study/pg/graduate-school/professional-skills/>

### 3.2.12 Letter Grades

Letter grades are produced by the assessors for the purposes of student feedback. For major pieces of coursework the letter grade is determined from a numerical mark,  $m$ , according to the following scheme:

A*	$m \geq 80\%$
A	$70\% \leq m < 80\%$
B	$60\% \leq m < 70\%$
C	$50\% \leq m < 60\%$
D	$40\% \leq m < 50\%$
E	$30\% \leq m < 40\%$
F	$m < 30\%$

## 3.3 Requirements for Passing the MSc

### 3.3.1 Classification of the MSc

0%-49%	Fail
50%-59%	Pass
60%-69%	Merit
70%-100%	Distinction

These percentages refer to the aggregate mark for the MSc.

**You must get at least 40% for every component to pass the MSc.**

This is a ruling passed by the Senate of the College in 2009. More precisely, the ruling states that if you get less than 50% in any component, then you will receive a compensated pass provided (i) your aggregate mark is at least 50% and (ii) you get no less than 40% in any component.

**If you get less than 40% in any component you will fail the entire MSc.**

### 3.3.2 Progression onto Year 2 for CDT Students on the 1+3 year programme

**In order to progress to year 2 of the CDT, MSc students must gain an aggregate mark of at least 60% in the MSc.**

If your aggregate mark is between 50% and 59% at the completion of the MSc, you will pass the MSc but you will cease to receive from the CDT a funding award for continuation onto the PhD.

### 3.3.3 Resits

There are no plans to hold any resits of examinations for the MSc.

### 3.3.4 How To Complain

Imperial College aims to give the highest specialised instruction and service to all its students, however, in some cases it recognises that students may not always be satisfied with the service that they have received. If you wish to raise a concern, you should first seek advice from your student representatives and raise the matter with the individual concerned. If you are not satisfied with the outcome, you should consult the College's Registry website which provides clear and consistent procedures that indicate how you can take your comments further:

<http://www.imperial.ac.uk/students/terms-and-conditions/appeals/>

## 3.4 Sutton Prize

A prize of £600 will be awarded to the student with the best overall performance in the MSc, as determined by the aggregate mark.

## 4. Board of Examiners

### 4.1 Board of Examiners

The Board of examiners for the MSc in Theory and Simulation of Materials includes:

- Dr Arash Mostofi
- Dr Johannes Lischner
- All academics teaching on the course in 2018-19

### 4.2 External Examiners



Prof Steven Kenny, Loughborough University

It is common for Master's level students to have some form of academic or social interaction with their external examiners at some point during or after their studies as well as during the assessment process itself.

It is inappropriate for you to submit complaints or representations directly to external examiners or to seek to influence your external examiners. Inappropriate communication towards an examiner would make you liable for disciplinary action.

A summary of External examiners reports from the previous academic year can be found here:



[www.imperial.ac.uk/staff/tools-and-reference/quality-assurance-enhancement/external-examining/information-for-staff](http://www.imperial.ac.uk/staff/tools-and-reference/quality-assurance-enhancement/external-examining/information-for-staff)

## 5. Location and Facilities

### 5.1 Location

Imperial has a number of campuses in London and the South East. All have excellent travel links and are easily accessible via public transport.

Your main location of study will be:

EPSRC CDT Suite  
4<sup>th</sup> Floor Library (access via the Sherfield Building only)  
South Kensington Campus

Imperial College's South Kensington Campus is located just south of the Royal Albert Hall in South Kensington. The nearest tube stations are South Kensington and Gloucester Road on the District, Circle and Piccadilly Lines.

Other CDT locations:

- The Department of Physics is located at the Blackett Laboratory, on the corner of Queen's Gate and Prince Consort Road (the entrance is on this road).
- The Department of Mechanical Engineering is in the City and Guilds Building, which can be accessed from the main entrance of the College on Exhibition Road.
- The Department of Chemistry is located on the White City Campus.
- The Department of Materials is based in the Royal School of Mines, the Bessemer Building and the Goldsmiths Building. These are on the corner of Exhibition Road and Prince Consort Road (the entrance is on this road).

#### 5.1.1 Maps

Campus maps and travel directions are available at:



[www.imperial.ac.uk/visit/campuses](http://www.imperial.ac.uk/visit/campuses)

#### 5.1.2 Accessibility

Information about the accessibility of our South Kensington Campus is available online through the DisabledGo access guides:



[www.disabledgo.com/organisations/imperial-college-london-2](http://www.disabledgo.com/organisations/imperial-college-london-2)

#### 5.1.3 Smoke-Free Policy

All Imperial campuses and properties are smoke-free. This means that smoking by staff and students is not permitted on or within 20 metres of College land. The policy covers all College properties, including student accommodation and sports grounds.



[www.imperial.ac.uk/smoke-free](http://www.imperial.ac.uk/smoke-free)



## 5.2 Facilities

### 5.2.1 Admin Support

The CDT Admin office is located in the EPSRC CDT Suite and is your first point of contact for any admin related queries. It is open 9am-5pm Monday to Friday.

The Department of Physics postgraduate office is located in room 316 Blackett Building.

### 5.2.2 Telephones

The general college number is 020 7589 5111 (+44 20 7859 5111 from overseas). The College operator may be obtained by dialling 0. Five-figure internal numbers may be dialled directly on the phone. All extension numbers prefixed with a 4 may be dialled directly by external callers using 020 7594-XXXX. Extension numbers prefixed with a 5 do not have the directly dialling facility. Use the college directory (<http://www.imperial.ac.uk/collegedirectory>) on the College website to find telephone numbers and offices of members of College. Microsoft Outlook also has contact details for the staff and students.

### 5.2.3 Photocopying, Printing, Scanning, Office Supplies

The printer in the EPSRC CDT Suite is accessed via the network. You can send printing jobs to the printer and then collect the output by swiping your college security card through the card reader on the front panel of the printer. The printer also acts as a photocopier and as a scanner. You can scan documents and send them to your email address. You can also request to use a guillotine, paper shredder and laminator via the CDT Administrators.

### 5.2.4 Mail

The CDT postal address is:

**CDT in TSM,**  
Imperial College London,  
**Blackett Building,**  
South Kensington Campus  
London,  
SW7 2AZ,  
UK

In general we do not encourage students to have mail sent to them at the CDT. But if it is necessary that something is sent to you at the CDT please inform the Senior Administrator, who will pass it on to you when it arrives.

### 5.2.5 Before you Arrive

Prior to arriving at Imperial College, you should have received joining instructions, a timetable and the details on the introductory lecture where you shall be given further details of the course, briefings and documents on your course and the CDT (such as safety information) and the opportunity to meet your colleagues. You are also encouraged to look at the web page for all new students at Imperial:

[www3.imperial.ac.uk/students/newstudents](http://www3.imperial.ac.uk/students/newstudents).

### 5.2.6 When you Arrive

MSc students will be sent an email inviting them to register online. The induction will take place on the first week day of Term 1. Laptops provided for all those taking the course will be distributed on the same day.

### 5.2.7 ID Cards

One of the very first things you need to do when you arrive is obtain an identity card. Instructions on how to obtain an ID card will be sent to you in the welcome packs. The ID card is essential for a number of purposes, including access to the Central Library. It is also used as a swipe card to get in and out of the EPSRC CDT Suite where the CDT is housed.

## 6. Working While Studying

If you are studying full time, the College recommends that you do not work part-time during term time. If this is unavoidable we advise you to work no more than 10–15 hours per week, which should be principally at weekends and not within normal College working hours.

Working in excess of these hours could impact adversely on your studies or health.

If you are here on a Tier 4 visa you can work no more than 20 hours a week during term time. Some sponsors may not permit you to take up work outside your studies and others may specify a limit.

If you are considering part-time work during term time you are strongly advised to discuss this issue with the Director or Cohort Mentor. If you are on a Tier 4 visa you should also seek advice from the International Student Support team regarding visa limitations on employment.

## 7. Health and Safety

You are responsible for looking after your own health and safety and that of others affected by your College-related work and leisure activities. You must:

- comply with all local and College policies, procedures and codes of practice and with the arrangements which the College has in place to control health and safety risks.
- ensure that your activities do not present unnecessary or uncontrolled risks to yourself or to others.
- attend appropriate induction and training.
- report any accidents, unsafe circumstances or work-related ill health of which you become aware to the appropriate person.
- not interfere with any equipment provided for Health and Safety.
- inform your supervisor or the person in charge of the activity in cases where you are not confident that you are competent to carry out a work or leisure activity safely, rather than compromise your own safety or the safety of others.

The College's Health and Safety Statement can be found at:



<http://www.imperial.ac.uk/safety/safety-by-topic/safety-management/health-and-safety-policy-statement/>

**Your Departmental safety contact is:**



Stefan Hoyle, 518 Sir Alexander Fleming Building

[s.hoyle@imperial.ac.uk](mailto:s.hoyle@imperial.ac.uk)

### 7.1 Safety

Although most of your MSc is class-based, you should be mindful of safety considerations at all times. All students are issued with the current version of the Blackett Laboratory Safety Booklet at the start of the MSc course, and all students are required to attend the Health and Safety Induction in the Physics Department and to complete the online Risk Assessment Foundation Training (RAFT). See <http://www.imperial.ac.uk/natural-sciences/departments/physics/safety> and [www3.imperial.ac.uk/safety](http://www3.imperial.ac.uk/safety) for more information.

#### 7.2.1 The College Safety Department

The Safety Department offers a range of specialist advice on all aspects of safety. This includes anything which you feel might affect you directly, or which may be associated with teaching, research or support service activities.

The College's activities range from the use of hazardous materials (biological, chemical and radiological substances) to field work, heavy or awkward lifting, driving, and working alone or late.

All College activities are covered by general health and safety regulations, but higher risk activities will have additional requirements.

The Safety Department helps departments and individuals ensure effective safety management systems are in place throughout the College to comply with specific legal requirements.

Sometimes the management systems fail, and an accident or a near-miss incident arises; it is important that we learn lessons from such situations to prevent recurrence and the Safety Department can support such investigations. All accidents and incidents should be reported online at:

 [www.imperial.ac.uk/safety](http://www.imperial.ac.uk/safety)

To report concerns or to ask for advice you should contact your programme director, academic supervisor or departmental safety officer in the first instance. You may also contact the Safety Department directly.

### 7.2.2 Occupational Health Requirements

The College Occupational Health Service provides services to:

- protect health at work
- assess and advise on fitness for work
- ensure that health issues are effectively managed

The Service promotes and supports a culture where the physical and psychological health of staff, students and others involved in the College is respected, protected and improved whilst at work.

 [www.imperial.ac.uk/occupational-health](http://www.imperial.ac.uk/occupational-health)

## 8. College Policies and Procedures

### 8.1 Regulations for Students

All registered students of the College are subject to the Regulations for Students, the College Academic and Examination Regulations and such other regulations that the College may approve from time to time.



[www.imperial.ac.uk/about/governance/academic-governance/regulations](http://www.imperial.ac.uk/about/governance/academic-governance/regulations)



[www.imperial.ac.uk/students/terms-and-conditions](http://www.imperial.ac.uk/students/terms-and-conditions)

### 8.2 Academic Feedback Policy

We are committed in providing you with timely and appropriate feedback on your academic progress and achievement, enabling you to reflect on your academic progress. During your study you will receive different methods of feedback according to assessment type, discipline, level of study and your individual need. Further guidance on the Policy of Academic Feedback can be found on the Academic Governance website:



<http://www.imperial.ac.uk/media/imperial-college/administration-and-support-services/registry/academic-governance/public/academic-policy/academic-feedback/Academic-feedback-policy-for-taught-programmes.pdf>

You should expect to receive feedback for assessed coursework related to the taught courses within two weeks of handing in the work. This feedback will usually be given at the next available rapid feedback session and will consist of a combination of a letter grade for your work, written comments on your work, and discussion during the rapid feedback session itself. Deadlines for assessed coursework and rapid feedback sessions are published in the Google Calendar timetable for the course.

### 8.3 Provisional Marks Guidance

Provisional marks are agreed marks that have yet to be ratified by the Board of Examiners. These results are provisional and are subject to change by the Board of Examiners. The release of provisional marks is permitted except in certain circumstances. Further information can be found in the Guidelines for Issuing Provisional Marks to Students on Taught Programmes:



<http://www.imperial.ac.uk/media/imperial-college/administration-and-support-services/registry/academic-governance/public/academic-policy/markings-and-moderation/Guidelines-for-issuing-provisional-marks-to-students-on-taught-programmes.pdf>

### 8.4 Late Submission Policy

You are responsible for ensuring that you submit your coursework assessments on time and by the published deadline. Any piece of assessed work which is submitted beyond the published deadline (date and time) would be classed as a late submission. Further guidance on Late Submission of Assessments can be found on the Academic Governance website:



<https://www.imperial.ac.uk/media/imperial-college/administration-and-support-services/registry/academic-governance/public/academic-policy/markings-and-moderation/Late-submission-Policy.pdf>

### 8.5 Academic Integrity

You are expected to conduct all aspects of your academic life in a professional manner. A full explanation of academic integrity, including information on the College's approach to plagiarism is available on the College website:



[www.imperial.ac.uk/student-records-and-data/for-current-students/undergraduate-and-taught-postgraduate/exams-assessments-and-regulations/plagiarism-academic-integrity--exam-offences](http://www.imperial.ac.uk/student-records-and-data/for-current-students/undergraduate-and-taught-postgraduate/exams-assessments-and-regulations/plagiarism-academic-integrity--exam-offences)

## 8.6 Academic Misconduct Policy and Procedures

It is important that you learn how to properly attribute and acknowledge the work, data and ideas of others. Plagiarism is scientific misconduct, and students whose assessments can be shown to contain plagiarism are subject to penalties as outlined in the College's Misconduct Policy and Procedures.



[www.imperial.ac.uk/about/governance/academic-governance/academic-policy/complaints-appeals-and-discipline](http://www.imperial.ac.uk/about/governance/academic-governance/academic-policy/complaints-appeals-and-discipline)

## 8.7 Appeal and Complaints Procedures

We have rigorous regulations in place to ensure assessments are conducted with fairness and consistency. In the event that you believe that you have grounds for complaint about academic or administrative services, or wish to appeal the outcome of an assessment or final degree, we have laid out clear and consistent procedures through which complaints and appeals can be investigated and considered:



[www.imperial.ac.uk/about/governance/academic-governance/academic-policy/complaints-appeals-and-discipline](http://www.imperial.ac.uk/about/governance/academic-governance/academic-policy/complaints-appeals-and-discipline)

## 8.8 Student Disciplinary Procedure

The College has the right to investigate any allegation of misconduct against a student and may take disciplinary action where it decides, on the balance of probabilities, that a breach of discipline has been committed. The general principles of the Student Disciplinary Procedure are available on the College website:



[www.imperial.ac.uk/admin-services/secretariat/college-governance/charters/ordinances/students/](http://www.imperial.ac.uk/admin-services/secretariat/college-governance/charters/ordinances/students/)

## 8.9 Intellectual Property Rights Policy

For further guidance on the College's Intellectual Property Rights Policy is available on the College website:



[www.imperial.ac.uk/students/enterprising-students/intellectual-property/](http://www.imperial.ac.uk/students/enterprising-students/intellectual-property/)

## 8.10 Use of IT Facilities

View the Conditions of Use of IT Facilities:



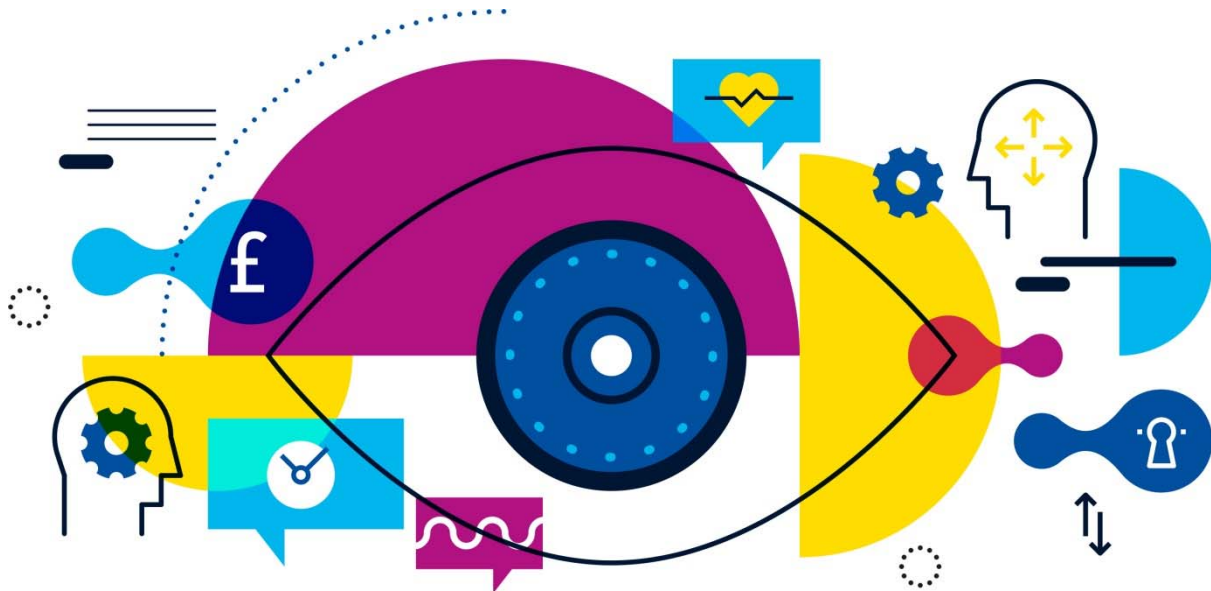
<http://www.imperial.ac.uk/admin-services/ict/self-service/computers-printing/staff-computers/conditions-of-use-for-it-facilities/>

## 9. Well-being and Advice

### 9.1 Student Space

The Student Space website is the central point for information on health and well-being.

 [www.imperial.ac.uk/student-space](http://www.imperial.ac.uk/student-space)



### 9.2 Departmental support and College tutors

Your Department has a system of academic and pastoral care in place to make sure you have access to the appropriate support throughout your time here. This includes:

#### Personal Postgraduate Tutor

The Department's Personal Postgraduate Tutor can offer pastoral support and advice. You can arrange to have a meeting with them at any time during your studies – what you discuss will be completely confidential.

If necessary they will direct you to an appropriate source of support.

#### Cohort Mentors

Each cohort of students has a mentor appointed to accompany them through the MSc and continues with those who stay on for the PhD. The role of the mentor is to be a point of contact for each student within a cohort throughout the course; to offer advice on the selection of options and projects; to help with career decisions; to be available for writing references; and to help with any matters of a non-academic nature that may arise. During the MSc, the cohort mentor also fulfils the crucial role of providing virtually instant feedback from MSc students about any aspect of their courses. This feedback is reported to the Operations Board, which normally meets weekly during term time. This has already proved to be an extremely effective way of identifying and solving problems before they become serious.

#### General

The academic support for the MSc students comes primarily from the course lecturers, the other academic staff associated with the CDT and project supervisors. The number of students on the MSc

course is normally a small enough group that they are actively encouraged to go directly to course lecturers and other staff with academic questions on an informal basis.

## Projects

For the MSc research projects, each student will have at least two supervisors allocated. For other projects such as the group projects, a member of academic staff will brief students about the work at the beginning of the project and thereafter advises the students whenever necessary.

## Writing and Communication Skills

There is written support material for writing skills and for the oral presentation of coursework – courses are arranged by the Graduate School and details will be given early in the course. Communication skills are assessed continuously throughout the course and students submit written work and give public oral presentations which are assessed and whose assessment counts towards their final degree result. Feedback to students is available on all submitted work and oral presentations.

## 9.3 Advice Services

The tutor system is complemented by a College-wide network of advice and support. This includes a number of specialist services.

### Careers Service

The Careers Service has strong links to your Department and you will have a named Careers Consultant and Placement and Internship Adviser who will run both group sessions and individual meetings within your Department. You can arrange to meet with your linked Careers Consultant or Placement and Internship Adviser either in your Department or centrally on Level 5 Sherfield where the Careers Service is based.

Visit the Career Service's website to:

- Book a careers appointment
- Find resources and advice on successful career planning



[www.imperial.ac.uk/careers](http://www.imperial.ac.uk/careers)

### Counselling and Mental Health

The Student Counselling and Mental Health Advice Service offers short-term counselling to all registered students. The service is free and confidential. Counsellors are available at the South Kensington, Hammersmith and Silwood Park Campuses.



[www.imperial.ac.uk/counselling](http://www.imperial.ac.uk/counselling)

### Financial support and tuition fees

If you've got any questions about student financial support (loans, scholarships and research council studentships, US and Canadian loans) then contact the Student Financial Support team:



020 7594 9014




[student.funding@imperial.ac.uk](mailto:student.funding@imperial.ac.uk)

If you suddenly find yourself in financial difficulties or experience an unexpected change in circumstances, you may be eligible to apply for emergency financial help through the Student Support Fund. The Fund offers a one-off payment of up to £2,000 to cover such emergencies as last minute accommodation and travel necessities, equipment and childcare. It does not have to be repaid.



 <http://www.imperial.ac.uk/students/fees-and-funding/financial-assistance/student-support-fund/>

For tuition fees queries, contact the Tuition Fees team:

 020 7594 8011

 [tuition.fees@imperial.ac.uk](mailto:tuition.fees@imperial.ac.uk)

### **Imperial College Union (ICU) Advice Centre**


Imperial College Union runs the Advice Centre independently of the College with advisers on hand to provide free, confidential, independent advice on a wide range of welfare issues including housing, money and debt, employment and consumer rights, and personal safety.


 [www.imperialcollegeunion.org/advice](http://www.imperialcollegeunion.org/advice)

### **Student Hub**

The Student Hub represents a single point of contact for all key administrative information and support. The Student Hub team can help you with enquiries about:

- Accommodation (including checking contracts for private accommodation)
- Admissions
- International student enquiries
- Research degrees
- Student financial support
- Student records
- Tuition fees

 Level 3, Sherfield Building, South Kensington Campus

 020 7594 9444

 [student.hub@imperial.ac.uk](mailto:student.hub@imperial.ac.uk)

 [www.imperial.ac.uk/student-hub](http://www.imperial.ac.uk/student-hub)

## **9.4 Health Services**

### **NHS Health Centre and finding a doctor**

Even if you're fit and healthy we recommend that you register with a local doctor (GP) as soon as you arrive in London. For help finding your nearest GP see the Student Space website:


 [www.imperial.ac.uk/student-space/here-for-you/find-a-doctor](http://www.imperial.ac.uk/student-space/here-for-you/find-a-doctor)

There is the Imperial College Health Centre on our South Kensington Campus which you may visit during clinic hours if you're feeling unwell. Students living within the practice catchment area are encouraged to register with the Centre.

 [www.imperialcollegehealthcentre.co.uk](http://www.imperialcollegehealthcentre.co.uk)

### **NHS Dentist (based in the Imperial College Health Centre)**

Imperial College Dental Centre offers a full range of NHS and private treatment options.

 [www.imperial.ac.uk/student-space/here-for-you/dentist](http://www.imperial.ac.uk/student-space/here-for-you/dentist)


## 9.5 Disability Support

### Disability Advisory Service

The Disability Advisory Service provides confidential advice and support for all disabled students and students with specific learning difficulties.

If you think you may have dyslexia or another specific learning difficulty but have never been formally assessed, the Disability Advisory Service offers initial screening appointments.

 Room 566, Level 5, Sherfield Building, South Kensington Campus

 020 7594 9755

 [disabilities@imperial.ac.uk](mailto:disabilities@imperial.ac.uk)

 [www.imperial.ac.uk/disability-advisory-service](http://www.imperial.ac.uk/disability-advisory-service)

### Departmental Disability Officers

Departmental Disability Officers are the first point of contact within your department. They can apply for additional exam arrangements on your behalf, and will facilitate support within your Department.

Your Disability Liaison Officer is **Dr Andrew Williamson**  
(Blackett 316, [andrew.williamson@imperial.ac.uk](mailto:andrew.williamson@imperial.ac.uk))

Andrew Williamson is your first point of contact within the Physics department and is there to help you with arranging any support within the department that you need. Andrew is also the person who will apply for Special Examination arrangements on your behalf. You need to contact him without delay if you think that you may need extra time or other adjustments for your examinations.

More information on Departmental Disability Officers is available at:

 [www.imperial.ac.uk/disability-advisory-service/support/ddos](http://www.imperial.ac.uk/disability-advisory-service/support/ddos)


More information on procedures for the consideration of additional exam arrangements in respect of disability is available at:

 [www.imperial.ac.uk/media/imperial-college/administration-and-support-services/registry/academic-governance/public/academic-policy/exam-arrangements-and-re-sits/Exam-arrangements-in-respect-of-disability.pdf](http://www.imperial.ac.uk/media/imperial-college/administration-and-support-services/registry/academic-governance/public/academic-policy/exam-arrangements-and-re-sits/Exam-arrangements-in-respect-of-disability.pdf)

## 9.6 Library and IT

### Information and Communications Technologies (ICT)

If you're having problems with technology (including computers, laptops and mobile devices), you can get help from ICT's Service Desk.

 020 7594 9000

 [www.imperial.ac.uk/ict/service-desk](http://www.imperial.ac.uk/ict/service-desk)

### Software shop

The Software shop offers a variety of general and subject specific software programs and packages for free or at a discounted price for Imperial students.

 [www.imperial.ac.uk/admin-services/ict/shop/software](http://www.imperial.ac.uk/admin-services/ict/shop/software)

### **Library services**

The Central Library at South Kensington is open around the clock pretty much all year. Make sure you find out who your departmental librarian is as they'll be able to help you find resources for your subject area. Also, don't forget to check out the Library's range of training workshops and our other campus libraries for access to specialist medicine and life sciences resources. Alongside these physical spaces and resources, the Library provides over 170,000 electronic books, journals and databases available both on and off campus and a free document delivery service to help you source books and articles from around the UK and the rest of the world:

 [www.imperial.ac.uk/library](http://www.imperial.ac.uk/library)

## **9.7 Religious Support**

The Chaplaincy Multi-faith Centre has chaplains from many different religions, as well as prayer rooms and information on places of worship. In addition, it runs meditation classes and mindfulness workshops for stress management. There is a student-run Islamic prayer room on campus and separate areas available for male and female Muslims.

 [www.imperial.ac.uk/chaplaincy](http://www.imperial.ac.uk/chaplaincy)

## **9.8 Support for International Students**

### **English language support**

The Centre for Academic English provides free in-sessional English courses for international students while they are studying. These include classes and workshops on academic language, social language, the four skills of reading, writing, listening and speaking, 1-1 consultations with a tutor to work on a piece of academic writing or an oral presentation, self-study resources in the VLE Blackboard, and the Conversation Project, which partners students with a native-speaker volunteer to practise social and conversational English.

 [www.imperial.ac.uk/academic-english](http://www.imperial.ac.uk/academic-english)

### **International Student Support team**

Students from outside the UK make up around half of our student population, so our International student Support team offers year-round support to help our international students settle into Imperial life. This includes UK visa and immigration advice and trips to different places of interest.

 [www.imperial.ac.uk/study/international-students](http://www.imperial.ac.uk/study/international-students)


## 10. Student Records and Data

The Student Records and Data Team are responsible for the administration and maintenance of the student records for all students studying at the College. This includes enrolments, programme transfers, interruption of studies, withdrawals and processing of examination entry for research degree students. The team also use this information to fulfil reporting duties to the Student Loans Company, Transport for London and the UKVI, as well as other external bodies.

The Team is responsible for the processing of student results and awards on the student record system as well as the production and distribution of academic transcripts and certificates of award.


The Student Records and Data Team produce a variety of standard document requests for both current and previous students including council tax letters, standard statements of attendance and confirmation of degree letters.

### Student records and examinations

 +44 (0)20 7594 7268

 [records@imperial.ac.uk](mailto:records@imperial.ac.uk)

### Degree certificates

 +44 (0)20 7594 8037

 [certificates@imperial.ac.uk](mailto:certificates@imperial.ac.uk)

## 11. Work-life Balance

The pace and intensity of postgraduate study at Imperial can be demanding so it's important to find time for outside interests.

### 11.1 Imperial College Union

The Union's range of 375+ student-led clubs, societies and projects is one of the largest of any UK university, opening up lots of ways for you to enjoy your downtime.

 [www.imperialcollegeunion.org/about-us](http://www.imperialcollegeunion.org/about-us)

### 11.2 Graduate Students' Union

The Graduate Students' Union is the postgraduate arm of Imperial College Union. The GSU works alongside the Imperial College Union President to ensure that the requirements of postgraduate students are catered for. It also organises a number of academic and social events during the year.

 [www.imperialgsu.com](http://www.imperialgsu.com)

### 11.3 Physical Activity Sport

Imperial College has a wide range of sports and activities on offer that cater for all standards and abilities. We have a recreational activity offer, competitive sports teams and an elite sport programme. We are dedicated to ensuring we have a diverse, inclusive and exciting offer for all.

After a one off induction fee of £40 you will get free use of the gym and swimming facilities on our campuses.

 [www.imperial.ac.uk/sport](http://www.imperial.ac.uk/sport)

## 12. Student feedback and representation

### 12.1 Feedback from Students

Your feedback is important to the CDT, the College and Imperial College Union. The primary mechanism for passing on your comments, concerns and suggestions to the Operations Board of the CDT is to speak to your Cohort Mentor. In the past this has proved to be a very effective way of tackling problems that have arisen during the course. The CDT Director is also happy to speak to you.

In addition, the following College-wide surveys give you regular opportunities to reflect on the shape of the courses and overall programme and your experience as a student in the CDT (see Section 13).

As a result of student feedback received in the past, the CDT has made major changes to the delivery of the course including the introduction of foundation courses and group projects, the coordination of coursework deadlines and changes to our assessment and feedback processes.

To find out more about any of these surveys or to see the results from previous surveys, visit:

<http://www.imperial.ac.uk/students/academic-support/student-surveys/pg-student-surveys/>

For further information on surveys please contact the Registry's Surveys Team at

[surveys.registrysupport@imperial.ac.uk](mailto:surveys.registrysupport@imperial.ac.uk)

### 12.2 Student Representation

Student Representatives are recruited from every department to gather feedback from students to discuss with staff. More information about the role, and instructions on how to become an academic representative, are available on the Imperial College Union (ICU) website.



[www.imperialcollegeunion.org/your-union/your-representatives/academic-representatives/overview](http://www.imperialcollegeunion.org/your-union/your-representatives/academic-representatives/overview)

### 12.3 Staff-Student Committee

Staff-Student Committees are designed to strengthen understanding and improve the flow of communication between staff and students and, through open dialogue, promote high standards of education and training, in a co-operative and constructive atmosphere. College good practice guidelines for staff-student committees are available here:



[www.imperial.ac.uk/about/governance/academic-governance/academic-policy/student-feedback](http://www.imperial.ac.uk/about/governance/academic-governance/academic-policy/student-feedback)

Please see section 1.6

## 13. Student Surveys

Your feedback is important to your department, the College and Imperial College Union.

Whilst there are a variety of ways to give your feedback on your Imperial experience, the following College-wide surveys give you regular opportunities to make your voice heard:

- PG SOLE lecturer/module Survey or departmental equivalent
- Student Experience Survey (SES)
- Postgraduate Taught Experience Survey (PTES)

The PG SOLE lecturer/module survey runs at the end of the autumn and spring terms. This survey is your chance to tell us about the modules you have attended and the lecturers who taught them.

For PG SOLE your lecturers will receive their individual numerical results and comments shortly after the survey closes. To make the most of your opportunity to give your feedback, please do not use offensive language or make personal, discriminatory or abusive remarks as these may cause offence and may be removed from the results. Whilst this survey is anonymous, please avoid self-identification by referring to personal or other identifying information in your free text comments.

The Student Experience Survey (SES) is another opportunity to leave your views on your experience. This survey will cover your induction, welfare, pastoral and support services experience.

The Postgraduate Taught Experience Survey (PTES) is the only national survey of Master's level (MSc, MRes, MBA and MPH) students we take part in. This is the only way for us to compare how we are doing against the national average and to make changes that will improve our Master's students' experience in future. PTES covers topics such as motivations for taking the programme, depth of learning, organisation, dissertation and professional development. PTES last ran in spring term 2018.

All these surveys are anonymous and the more students that take part the more representative the results so please take a few minutes to give your views.

The Union's "You Said, We Did" campaign shows you some of the changes made as a result of survey feedback:

 [www.imperialcollegeunion.org/you-said-we-did](http://www.imperialcollegeunion.org/you-said-we-did)

If you would like to know more about any of these surveys or see the results from previous surveys, please visit:

 [www.imperial.ac.uk/students/academic-support/student-surveys/pg-student-surveys](http://www.imperial.ac.uk/students/academic-support/student-surveys/pg-student-surveys)

For further information on surveys, please contact the Registry's Surveys Team at:

 [surveys.registrysupport@imperial.ac.uk](mailto:surveys.registrysupport@imperial.ac.uk)

## 14. And finally

### 14.1 Alumni Services

When you graduate you will be part of a lifelong community of over 190,000 alumni, with access to a range of alumni benefits including:

- discounts on further study at the College and at Imperial College Business School
- alumni email service
- networking events
- access to the Library and online resources
- access to the full range of careers support offered to current students for up to three years after you graduate
- access to our Alumni Visitor Centre at the South Kensington Campus, with free Wifi, complimentary drinks, newspapers and magazines, and daytime left luggage facility

Visit the Alumni website to find out more about your new community, including case studies of other alumni and a directory of local alumni groups in countries across the world.



[www.imperial.ac.uk/alumni](http://www.imperial.ac.uk/alumni)

### 14.2 Opportunities for Further Study

After you have completed the MSc in Theory and Simulation of Materials, most students continue on to a PhD within the TSM CDT. However, the MSc will provide knowledge and skills that will be useful to a wide range of opportunities within and external to academia. Previous graduates have gone on to further study at Imperial and elsewhere – see the Director's induction talk for examples.

### 14.3 And When You Leave Imperial...

Once your studies with the CDT have ended please ensure you:

- Return all keys, ID card, books and other College material.
- Provide details of how you can be contacted as we like to stay in touch with our Alumni and may need to contact them for information on occasion
- Provide your details of your first destination after the CDT.

If, as will be the case for most of you, you are staying on for the further three years of the CDT then you should retain your ID card and any other College material for the duration of your PhD. During the three years of your PhD training you will retain access to the EPSRC CDT suite and you will be welcome to use its facilities, although you will not retain a desk space.



## Appendix 1      Synopses of courses

The following brief descriptions of the content of the courses are indicative and changes may be made by the lecturer before each course starts. The descriptions given here may not always match the College Prospectus, since the Prospectus is prepared up to 18 months before a course is given.

# Compulsory core courses

# Mathematics for the Theory of Materials (MTM1 and MTM2)

Dr Gunnar Pruessner (GP)

24 one-hour lectures and 7 rapid feedback sessions in Term 1

*Items in italics are pre-requisite knowledge.*

- I. **Vector Spaces & Tensors [3 lectures & 1 RF]**. Definition of a vector space; dimensionality, orthogonality, linear dependence. Reminder of eigenvectors, eigenvalues and normal modes. Tensor algebra, suffix notation, rank. Transformation law. Tensor fields. Representation of grad, div and curl. Principal axes and diagonalisation. Representation quadric. Stationary property of eigenvalues. Neumann's principle. Heat flow in anisotropic crystals as an example. (*Pre-requisite knowledge: vector and matrix algebra; special types of matrix, eg, unitary, Hermitian, etc.; determinants; linear equations; eigenvectors, eigenvalues, normal modes*).
- II. **Green's Functions [3 lectures & 1 RF]**. Dirac delta function. Variation of parameters method for inhomogeneous ODEs. Green's functions for initial value and boundary value problems.
- III. **Hilbert Spaces [3 lectures & 1 RF]**. Definition of a Hilbert space; dimensionality, orthogonality, linear dependence, Wronskian. Sturm-Liouville Theory; self-adjoint operators, eigenfunctions, eigenvalues, weight function. Eigenfunction expansions, completeness. Examples of orthogonal functions to include Bessel functions, spherical harmonics and Legendre polynomials, including solution of Laplace's equation in spherical polar coordinates by separation of variables and series solution of Legendre's equation.
- IV. **Integral Transforms [3 lectures & 1 RF]**. Continuous Fourier transforms: Parseval's theorem and convolution theorem; bandwidth theorem and connection to quantum mechanics; application to Fraunhofer diffraction and heat diffusion. Laplace transforms: convolution theorem; application to ordinary differential equations. (*Pre-requisite knowledge: Fourier series, orthogonality of cos and sin, Gibbs phenomenon, Parseval's theorem and Bessel's inequality for Fourier series, odd and even functions, Kronecker delta*).
- V. **Complex Analysis and Contour Integration [7 lectures & 2 RF]**. Functions of a complex variable. Cauchy-Riemann relations, analytic functions, Cauchy's theorem, Laurent's theorem. Order of poles. Residue theorem. Principal values and the Kramers-Kronig relation. Jordan's lemma. Contour integration. Inverse integral transforms; Bromwich integral. (*Pre-requisite knowledge: complex numbers; Argand diagram; modulus and argument; Cartesian and polar form;  $z^y$ , with  $y$  not necessarily an integer; multi-variate real calculus; vector calculus; line integration; Taylor and Maclaurin series; Laplace transform; Dirac delta function.*)
- VI. **Calculus of Variations [5 lectures & 1 RF]**. Lagrange multipliers. Functionals and functional differentiation. Local, non-local, and semi-local functionals. Euler-Lagrange equations. Application to classical mechanics. Euler-Lagrange equations for multiple dependent/independent variables. Variational principles. Rayleigh-Ritz methods; connection to Sturm-Liouville problems and constrained minimisation. Application to solving the Schroedinger equation. (*Pre-requisite knowledge: multi-variate real calculus; vector calculus; line, area and volume integration, Dirac delta function.*)

## Continuous Assessment

- For sections I to IV, there are four problem sheets, one per week, with one long question assessed each.
- For sections V and VI, there are three problem sheets, one per week, with 4-5 assessed problems each.
- The problem sheets also contain other problems that are not assessed.

# Equilibrium in Materials (EQM1)

Dr Stefano Angioletti-Uberti

16 one-hour lectures and 4 rapid feedback sessions in Term 1

## Macroscopic Approach: Thermodynamics

1. Elements of (Bulk/Homogeneous) Thermodynamics
  - a) Basic concepts
  - b) The laws of thermodynamics
  - c) The fundamental equation & equations of state
  - d) Maxwell relations
2. External Constraints, Thermodynamic Potentials and Important Relations
  - a) Spontaneous processes
  - b) From entropy to free energy: constraints and the Legendre transform
  - c) Helmholtz and Gibbs free energy
  - d) Open systems at constant temperature: Grand potential
3. Free energy and phase behaviour
  - a) Stability of a single phase
  - b) Equilibrium between two phases
  - c) Computing coexistence and phase diagrams
  - d) Gibbs-Duhem equation and Gibbs "phase rule"
  - e) Equilibrium in chemical reactions

## Microscopic Approach: Statistical Mechanics

1. Introduction to statistical mechanics
  - a) The "ergodic" hypothesis
  - b) Boltzmann entropy and the micro-canonical partition function
  - c) Partition functions of different ensembles
  - d) Linking statistical mechanics to thermodynamics
  - e) Fluctuations
2. Statistical mechanics of simple systems
  - a) Ideal gas
  - b) Non-ideal gas 1: the virial expansion
  - c) "Widom insertion" and the excess chemical potential
  - d) Ideal and non-ideal alloys: the regular solution model
  - e) Polymer mixtures and the Flory-Huggins theory
  - f) Perturbation theory and the Gibbs-Bogoliubov relation
  - g) Mean-field theory of magnetization
  - h) Adsorption of gas on surfaces

*Additional optional topics to be covered if time allows:*

- **Equilibrium in Non-Homogeneous Systems**
  - Elements of (classical) density functional theory
  - Polymer brushes

## Recommended Textbooks

- H. B. Callen, Thermodynamics and an Introduction to Themostatistics 2nd edition (New York, Wiley, 1985).
- D. Chandler, Introduction to Modern Statistical Mechanics (Oxford University Press, 1987).
- L. Peliti, Statistical Physics in a Nutshell (Princeton University Press)

## **Course Administration and Learning Support**

*Lecture notes:* Most of the material is extensively covered in the suggested textbooks but some notes will also be provided.

*Homework and Rapid Feedback:* Problem sets will be assigned each week. They will be used to both reinforce the main points of the lectures as well as to allow the student to go more in depth on certain topics as well as to carry out explicit calculations on certain problems of interests. Solutions of (selected) problems will be covered in separate weekly problem-solving sessions.

*Office hours:* Office hours can be used as an opportunity to meet and discuss with the lecturer any aspect of the course. These will be announced at the beginning of the first lecture.

# Transformations of Materials (TM1)

Professor Peter Haynes

## 16 one-hour lectures and 4 rapid feedback sessions in Term 1

The aim of this course is to cover the background theory necessary for understanding phase transformations in materials. It will therefore focus primarily on theoretical concepts, but illustrate them by application to real materials wherever possible. Thermodynamics applies to systems in equilibrium e.g. we can use it to calculate the relative stability of two phases. However in order to calculate the rate with which one phase will transform into another we need to study kinetics, which are often determined by diffusion processes. This is crucial for understanding how the processing of a material affects its microstructure, which in turn determines its properties. The concepts taught in this course will be picked up and applied to specific types of transformations in the advanced course TM2.

The continuous assessment for this course will take the form of four assessed problem sheets containing a total of ten questions. One question from each sheet will be selected for assessment.

### Prerequisites

This course assumes familiarity with the material covered in EQM1.

### Synopsis

#### 0. Microstructure

Examples of different microstructures and their influence on materials properties; control by processing and the central role of kinetics.

#### 1. Driving forces and fluxes for diffusion (PES chapter 1, BAC chapters 2 & 3)

- a. The role of Gibbs free energy in thermodynamics (equilibrium condition  $dG = 0$ ) and kinetics (activation free energy and Arrhenius laws).
- b. Regular solution model of binary substitutional alloy: derivation of the free energy of mixing for a random alloy (configurational entropy from Stirling's approximation, enthalpy from the quasichemical approach); connection between plots of  $G$  versus composition and binary phase diagrams for both exothermic and endothermic mixing at high and low temperatures; miscibility gap, common tangent construction and lever rule to determine equilibrium composition; nucleation versus spinodal decomposition; chemical potentials and their interpretation using plots of  $G$  versus composition; departure from ideal behaviour due to ordering or clustering of atoms, activities and activity coefficients, Henry's law and Raoult's law for dilute solutions.
- c. Driving forces for diffusion: fundamental role of chemical potential gradient (illustrated using  $G$  versus composition plots) and the possibility of 'uphill' diffusion against a concentration gradient; additional driving forces from interfacial energy (Gibbs-Thomson effect), electrostatic potential gradient for charged species and stress (formation of Cottrell atmospheres and creep)
- d. Fluxes and conjugate forces: derivation of Fick's first law and the analogy with current flow (Ohm's law) and heat flow (Fourier's law); coupling of fluxes and Onsager's symmetry principle as seen in the Seebeck and Peltier effects and electromigration; network constraints and vacancies.

#### 2. The diffusion equation (PES chapter 2, BAC chapters 4 & 5, BB)

- a. Derivation and simplification of the diffusion equation from Fick's first law and conservation of matter.
- b. Steady-state solutions (harmonic functions) for planar, cylindrical and spherical geometries.
- c. Linearity of the diffusion equation: superposition and the uniqueness theorem for the diffusion equation (proof not required).
- d. Separation of variables: solution of the diffusion equation in a finite spatial domain; treatment of the initial condition using orthogonal functions (e.g., Fourier series).
- e. Fundamental solution: derivation for the infinite spatial domain using integral transforms; superposition of solutions for the semi-infinite spatial domain by analogy with the method of images in electrostatics; derivation of error function solutions by superposition of point sources.

- f. Scaling: characteristic diffusion length and solution method for a 1D semi-infinite spatial domain through conversion to an ordinary differential equation; re-derivation of error function solutions; re-derivation of the fundamental solution by superposition.
  - g. Precipitate growth: Stefan (moving) boundary conditions; solution for planar and spherical geometries (recall of the form of the solution is not required).
- 3. Atomic mechanisms for diffusion in solids** (PES chapter 2, BAC chapters 7–9, BB)
- a. Random walks: derivation of diffusivity in  $d$  dimensions; re-derivation of fundamental solution in one dimension.
  - b. Interstitial diffusion: octahedral interstitial sites in bcc and fcc, re-derivation of Fick's first law for cubic lattices, migration free energy barrier and jump rate.
  - c. Substitutional diffusion in a pure metal: vacancy mechanism: derivation of equilibrium vacancy, activation energy for diffusion and its correlation with melting temperature; direct exchange, ring and interstitialcy mechanisms.
  - d. Substitutional diffusion in a binary alloy: Kirkendall effect; derivation of Darken's equations; dislocation kinks as sources/sinks of vacancies.
  - e. High-diffusivity paths: grain boundaries and dislocations; estimation of their relative importance at high and low temperatures relative to lattice diffusion.
- 4. Interfaces and microstructure** (PES chapter 3, BAC appendix B)
- a. Classification of interfaces: sharp *versus* diffuse; singular, vicinal and general; homophase *versus* heterophase; coherent, semi-coherent and incoherent.
  - b. Interfacial free energy: effect on nucleation;  $\gamma$ -plot and Wulff construction.
  - c. Instabilities in solidification fronts: undercooling in pure liquids and constitutional supercooling of alloys; Mullins-Sekerka linear stability analysis for spherical interfaces.

#### References and recommended reading

PES – D. A. Porter, K. E. Easterling, and M. Y. Sherif, *Phase Transformations in Metals and Alloys*, Third Edition (Taylor & Francis, 2009) – an accessible text at the level of a final year undergraduate or Master's course, a good place to start.

BAC – R. W. Balluffi, S. M. Allen, and W. C. Carter, *Kinetics of Materials* (Wiley, 2005) – an advanced graduate text that contains much detail but also an invaluable set of worked problems.

BB – additional material on Blackboard site

## Electronic Structure of Materials (ESM1)

Johannes Lischner (8 lectures) and Paul Tangney (8 lectures)

16 one-hour lectures and 4 rapid feedback sessions in Term 1

The aim of this course is to introduce students to some fundamental concepts of the electronic structure of materials. The course consists of two parts: i) concepts for understanding interacting many-electron systems (taught by Paul Tangney) and ii) applications of electronic structure theory to materials (taught by Johannes Lischner).

### Prerequisites:

The course assumes familiarity with basic concepts of quantum mechanics, such as operators, wave functions, solutions of the Schrödinger equation for simple systems (free particle, simple harmonic oscillator, hydrogen atom).

A useful reference is "A Cavendish Quantum Mechanics Primer" from M. Warner and A.C.H. Cheung, Periphyseos Press.

### Synopsis:

**Part 1: Making quantum mechanics tractable for many-electron systems: the simplifying assumptions and approximations (PT).**

#### Statement of the problem.

Many electrons and many nuclei; Schrödinger's time-dependent equation and the meaning of the wave function; stationary states; time-independent Schrödinger equation; variational principle; Hohenberg-Kohn theorems; observables  $\langle \Psi | \hat{O} | \Psi \rangle = O[n]$ .

#### Mathematically separating electrons and nuclei

Adiabatic and Born-Oppenheimer approximations; classical nuclei; Hellman-Feynman theorem.

#### Calculating electronic properties using the wave function, $\Psi$ :

Meanings of "exchange" and "correlation"; Hartree approximation; Hartree-Fock approximation; Beyond Hartree-Fock – what would an exact solution look like? Systematic improvements to Hartree-Fock.

#### Calculating electronic properties using the density, $n$ :

Density functional theory (DFT); Kohn-Sham approach to partitioning the total energy and calculating the ground state density; the Local Density Approximation (LDA); successes and failures of DFT; justification for (*quasi*-) independent electron models of materials.

### **Part 2: Using quantum mechanics to compute the properties of materials (JL).**

#### Using quantum mechanics to solve mysteries of metals:

Failure of classical statistical mechanics to explain specific heat of metals; Sommerfeld theory of metals; periodic boundary conditions; total energy; density of states and bulk modulus of the electron gas; Sommerfeld expansion.

#### Electrons in crystals:

Crystal lattices; Wigner-Seitz cell; periodicity; lattice Fourier series; Schrödinger's equation in a periodic potential; Bloch's theorem; crystal momentum; the nearly-free electron gas; metals; semiconductors and insulators; the role of symmetry.

#### From atoms to crystals:

Core and valence electrons; many-electron atoms; Aufbau principle and the periodic table; shell structure of atoms; electronegativity; bonding (van der Waals, ionic, covalent, metallic, hydrogen); tight-binding method; one-dimensional chain of hydrogen atoms.



### **Beyond the rigid ion approximation:**

Failures of the rigid ion approximation; vibrations of a chain of atoms; physics underlying the Lennard-Jones potential; small deviations from equilibrium; normal modes; speed of sound; vibrations of a three-dimensional crystal; acoustic and optical modes; quantum theory of lattice vibrations; phonons; specific heat; Debye temperature.

### **Continuous assessment**

There will be four assessed problem sets.

### **Books**

F. Giustino, *Materials Modelling using Density Functional Theory*, Oxford (2014). This is a new book that was written with materials scientists in mind. It covers most of the topics taught in this course.

M. L. Cohen and S. G. Louie, *Fundamentals of Condensed Matter Physics*, Cambridge University Press (2016). This is a very new book on condensed matter physics, which also explains the basics of density functional theory and Hartree-Fock theory.

N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, Thomson Learning Inc. (1976). A classic textbook of solid-state physics. A good source for band theory, phonons, tight binding, etc.

E. Kaxiras, *Atomic and Electronic Structure of Solids*, Cambridge University Press (2008). Much of the material in this book is also presented in Cohen and Louie or Ashcroft and Mermin, but the presentation is different and may appeal to some students. The appendices are useful because they succinctly cover some of the important background material.

A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, Dover Publications Inc. (1996). This book introduces electronic structure theories for many-electron systems in atoms and molecules, such as Hartree-Fock, configuration interaction and coupled cluster theory.

# Classical Field Theory of Materials (CFTM1)

Professor Adrian Sutton

16 one-hour lectures and 4 rapid feedback sessions in Term 1

## Synopsis

- Structural vs. functional materials. Mechanical properties are determined by physics across length and time scales.
- Defects in crystals: point, linear and planar defects.
- The geometry of the elastic field: displacement vector, distortion tensor, symmetric and antisymmetric components corresponding to strains and rotations respectively. Force and stress, and the stress field. The symmetry of the stress tensor. Invariants of the stress tensor. Linear elasticity, Hooke's law and the elastic constants as material parameters. Voigt (engineering) notation. The three independent elastic constant of cubic crystals and two of isotropic materials, and elastic anisotropy ratio in cubic crystals. The energy of the elastic field.
- The equilibrium condition for the stress field and body forces. Surface tractions. Application of Gauss's theorem to determine the average stress tensor within a body.
- The misfitting sphere as a model of point defects. Elastic solution in an infinite isotropic medium and in a sphere of finite radius.
- The elastic Green's function.
- Application of the elastic Green's function to point defects with non-spherical symmetry, and connection with atomistic simulation.
- The nature of plastic deformation of crystals: slip. Frenkel's analysis of slip of entire planes: the need for dislocations. Schmid's law. The Burgers vector, edge, screw and mixed dislocations, dislocation sources, stacking faults, perfect and partial dislocations, Lomer-Cottrell locks, pile-ups and the Hall-Petch relation, low angle grain boundaries. The isotropic elastic field of a straight screw dislocation derived heuristically.
- Application of the elastic Green's function to dislocations: Volterra's formula, Mura's formula.

## Continuous assessment

2 or 3 problems and/or short essays will be set for each of the 4 rapid feedback sessions.

## Books

The most recent draft of Adrian Sutton's own book will be distributed electronically, and will form the principal text on which the course is based. This book is still being developed.

### *Elasticity*

- C Teodosiu, *Elastic models of crystal defects*, Springer (1982). This is an excellent book on elasticity oriented towards defects in solids. It has just been brought back into print and three copies have been ordered for the CDT library. It is a good book to learn from because it is rigorous without being pedantic, and it is a book you will return to in later years because it is a mine of information.

### *Dislocations*

- D Hull and D J Bacon, *Introduction to Dislocations*, Pergamon (1992). This is a very readable introduction to dislocations in solids.
- J Weertman and J R Weertman, *Elementary dislocation theory* OUP (1992). Another very readable introduction to dislocations in solids.

### *Elasticity, defects*

- A H Cottrell, *The mechanical properties of matter*. This is a very clear introduction to the subject, written by possibly the finest metallurgist of all time.

### **More advanced books**

- R J Asaro and V A Lubarda *Mechanics of of solids and materials*, Cambridge University Press, (2010). This is a comprehensive and fairly advanced text.
- T Mura *Micromechanics of defects in solids*, Kluwer (1991). This is an advanced text, but very useful and well written, and directly related to Eshelby's work.
- J D Eshelby, *The continuum theory of lattice defects*, Vol 3 of Solid State Physics, eds. F Seitz and D Turnbull, p.79 (1956), in *Collected works of J D Eshelby* eds. X Markenscoff and A Gupta, Springer (2006). Eshelby is a towering giant in this field. His papers are very deep and beautifully written. You could spend a lifetime studying the 58 papers in his collected works.
- J P Hirth and J Lothe, *Theory of dislocations*, Krieger (1992). This is an advanced treatise on dislocations in solids. Chapter 2 is a good introduction to Elasticity.

## Methods of Simulating (MSM1 and MSM2)

Prof Daniele Dini (organiser), Dr Andrew Horsfield, Dr Johannes Lischner, Dr Paul Tangney

32 hours of lectures and classes in Term 2

### Course Overview

There will be eight topics, each lasting one week. For each topic there will be two hours of lecture and two hours of problem solving / feedback. The topics and associated exercises will be:

Topic	Lecturer	Exercises	Homework
1. Introduction	Daniele Dini & Andrew Horsfield	Multiscale Simulations Overview & MATLAB program	N/A
2. Density functional theory	Johannes Lischner	Hydrogen atom	1
3. Energy landscapes	Paul Tangney	Static relaxation calculations	2
4. Molecular dynamics	Paul Tangney	Molecular dynamics simulations	
5. Kinetic Monte Carlo	Andrew Horsfield	Hopping of disks between bins	3
6. Metropolis Monte Carlo	Andrew Horsfield	1D equilibration	
7. Finite Elements	Daniele Dini	1D and 2D finite elements of simple engineering structures	4
8. Crystal Plasticity	Daniele Dini	Plasticity in crystalline structures	

### Assessment

- Four problem sets (one per lecturer) based on the exercises. This is worth 70%.
- An eight minute prepared talk by each student. The students will be given a choice of four topics to choose from, of which they choose one. The presentations will take place in the first week of Term 3. This is worth 30%.
- The topics for the talks are:
  - Using kinetic Monte Carlo to solve the diffusion equation. Discuss the simulations you performed (NOT including the advanced tasks), offering answers to the questions asked in the description of the exercises.
  - Computing the ionization potential of atoms with DFT. Discuss how DFT can be used to compute total energies and ionization potentials of atoms and describe the results obtained in class and in the assessed problem. What are the problems of this approach, what are its merits?
  - Molecular Dynamics simulation of polymer dynamics. Discuss Langevin Dynamics and what it can tell you about the dynamics of a polymer in solution.
  - Finite Element Method for Solids and Structures. Discuss the steps required to build up a 2D finite element model to calculate displacement and forces in bodies subjected to external loads. Refer to the simulations you performed and discuss real life applications.

### Contact details

Name	E-mail	Phone
Daniele Dini	<a href="mailto:d.dini@imperial.ac.uk">d.dini@imperial.ac.uk</a>	4-7242
Andrew Horsfield	<a href="mailto:a.horsfield@imperial.ac.uk">a.horsfield@imperial.ac.uk</a>	4-6753
Johannes Lischner	<a href="mailto:j.lischner@imperial.ac.uk">j.lischner@imperial.ac.uk</a>	4-9949
Paul Tangney	<a href="mailto:p.tangney@imperial.ac.uk">p.tangney@imperial.ac.uk</a>	4-8155

## Syllabus

### Introduction

Overview of what computer modelling of materials is for, and can achieve. Survey of length and time scales and the methods appropriate to each. Introduction to MATLAB with practise exercises.

### Density-functional theory

Atomic length and time scales; fundamental theorems of density-functional theory; deriving the Kohn-Sham equations; approximate DFT: the local density approximation and beyond; exchange-correlation hole; spin polarization; Kohn-Sham equation for atoms; spherical symmetry; pseudopotentials; computing total energies and ionization potentials of atoms; the problem of self-interaction.

### Energy landscapes

Describing energy landscapes: the potential energy function  $U(\{R\})$ ; ab initio methods (quantum mechanics for electrons and the connection to N-body classical potential energy functions for ions, Born-Oppenheimer approximation); pair potentials (Lennard-Jones, Born-Mayer); semiconductors and metals (angular terms, bond-order potential, embedded-atom); molecular mechanics; induced dipoles in ionic systems; parameterization and force fitting. Exploring energy landscapes: molecular dynamics (basic concept, Verlet algorithm); finding minima (steepest descent, conjugate gradients, Newton methods).

### Molecular Dynamics

Tricks of the trade: periodic boundary conditions; Ewald summation; neighbour lists; thermostats; barostats. Case studies to illustrate: Accessible time and length scales; Fluctuations and their explanation in terms of basic statistics; Correlation functions; Exploiting the fluctuation-dissipation theorem; Using atomistic simulations to provide a) ideas and b) numbers (with the help of DFT).

### Kinetic Monte Carlo

Slow processes and local equilibrium; master equation; detailed balance. Link to diffusion equation and chemical rate equations. N-Fold Way Monte Carlo algorithm. Example applications.

### Metropolis Monte Carlo

Review of statistical mechanics; computing averages. The Metropolis algorithm (NVT); Extensions to other ensembles (NPT,  $\mu$ VT). Free energy calculations. Example applications.

### Finite elements

Basic principles of Finite Elements for frames and continua; 1D Finite Element definition, 2D local and global coordinates; Linear shape function in 1D; Determination of Forces, Stress and Strain and Strain Energy; 1D Example application. 2D beam elements; Constant Strain Triangle; Jacobian matrix and Stiffness matrix; Assembly of matrix equation of equilibrium.

### Crystal plasticity

Relevant tensors and continuum mechanics review. Slip systems review. Homogeneous deformation on a single slip system. Generalisation to multiple slip systems. Linear independence requirement for arbitrary plastic deformation. Resolved shear stress. Hardening and the single crystal flow rule. Theorems on uniqueness of stress, strain and slip rates; max/min principals. Determining slips from plastic strains. Overview of small strain computational implementation and model results.

# Advanced core courses

## Equilibrium in Materials (EQM2)

Professor Mike Finnis

8 hours of classes in Term 2

**Prerequisites:** Core courses EQM1 and TM1

**Continuous assessment:**

- 3 problem sheets to be handed in

**Examination:**

- Viva voce examination

The overarching theme of this module will be 'Atomistic Thermodynamics', or modern approaches to calculating thermodynamic properties by studying the energies and dynamics of collections of atoms, either quantum mechanically or classically. We shall study two broad themes as described below. Besides the sources noted below, my 2013-14 Lecture Notes for EQM and S&I could be useful.

**Indicative syllabus** (time may not permit all of the topics to be covered)

### 1. The thermodynamics of planar, line and point defects:

We shall study a rigorous thermodynamic treatment of surface energy, surface tension, segregation and other properties that play no part in the usual thermodynamics of bulk materials, with particular emphasis on how they can be calculated with atomistic models. The extension to line defects (dislocations) and point defects (e.g. vacancies) will be studied.

1.1 Cahn, J. Thermodynamics of Solid and Fluid Interfaces, in "Interfacial Segregation", W.C.Johnson, J.M.Blakely, American Society for Metals, Ohio (1977).

1.2 Sutton, A.P. and R.W. Balluffi, Interfaces in Crystalline Materials. 1995, Oxford: Clarendon. (available in paper back)

1.3 Finnis, M.W., Accessing the Excess: an atomistic approach to excesses at planar defects and dislocations in ordered compounds. Physica Status Solidi A, 166, 397-416 (1998).

### 2. CALPHAD: Calculation of PHase Diagrams:

It is a major concern in the design of new materials and their production and characterisation to understand the occurrence and stability of all kinds of solid phases that might be formed. In the past this process has been very empirical, but increasingly electronic structure calculations (Density Functional Theory – DFT) are providing data that is inaccessible to experimentalists. This topic is about the principles of modern phase diagram calculation. A particularly general problem we shall address is how to calculate the free energy up to the melting point of a simple element or compound, which includes contributions from vibrations, electronic excitations and point defects.

2.1 Hillert, M. Some viewpoints on the use of a computer for calculating phase diagrams, Physica B, vol 103, 31-40, (1981).

2.2 Physica Status Solidi B, vol 251, (2014) (a special issue)

2.3 Grabowski, B., L. Ismer, T. Hickel and J. Neugebauer, Ab initio up to the melting point: Anharmonicity and vacancies in aluminum. Physical Review B, 79, 134106 (2009)

2.4 Monserrat, B., N.D. Drummond, R.J. Needs, Anharmonic vibrational properties in periodic systems: energy, electron-phonon coupling, and stress. Physical Review B, 87, 144302-1-10, (2013)

# Transformations of Materials (TM2)

Dr Chris Gourlay

## 8 hours of classes in Term 2

This course builds an understanding of phase transformations as the origin of microstructure in materials.

### Prerequisites:

- Transformations of Materials Part 1
- Equilibrium in Materials Part 1

### Continuous assessment:

- Presentation
- Problem sheets

### Examination:

- Viva voce examination

### Indicative syllabus (time may not permit all of the topics to be covered)

The aim of this course will be to study the underlying theoretical concepts associated with the following topics in order to connect them with practical computational methods for simulating transformations in materials.

#### 1. Nucleation

- a. Classical nucleation theory (homogeneous and heterogeneous)
- b. Stochastic and deterministic nucleation
- c. Grain refinement (nucleant potency and the role of solute)

Key questions include: Can we control grain size in a phase transformation? What makes a potent nucleant? Does easy nucleation mean many nucleation events? What is the link between nucleation undercooling and grain size? How does nucleation in a liquid compare with nucleation in a solid? How could you model nucleation?

#### 2. Eutectic and eutectoid transformations

- a. Jackson-Hunt theory of regular eutectic growth (diffusion versus curvature)
- b. Growth at the extremum and spacing adjustment mechanisms
- c. Influence of faceting on eutectic growth

Key questions include: Why are eutectic spacings usually about 1-10 $\mu\text{m}$ ? Why is there no general theory for eutectic growth in real engineering alloys? Why is a theory of eutectoid growth a challenge?

#### 3. Martensitic transformations

- a. Diffusionless transformations
- b. Martensitic transformation in carbon steel
- c. Shape memory effect

Key questions include: What determines whether atomic motion is 'civilian' and 'military'? What are the conditions required for a Martensitic transformation? Why is the crystallography of Martensite transformations important?



# Electronic Structure of Materials (ESM2)

Dr Arash Mostofi

8 hours of classes in Term 2

**Prerequisites:**

- Electronic Structure of Materials Part 1

**Continuous assessment:**

- 1 set of hands-on practical computational exercises associated with modules 1-2
- 1 set of hands-on practical computational exercises associated with module 3
- 1 written essay associated with module 4

**Examination:** Viva voce examination

**Synopsis**

This course builds upon the material covered in the core course ESM1. The overall aim is for students at the end of this course to be confident about the background theory and practical application of modern electronic structure methods for calculating the ground and excited state properties of materials.

The course is structured in four modules. The reading for each module is meant to act as a springboard for further self-study.

**1. Energy bands in solids [1 session]** Crystal lattices; Bloch's theorem; crystal momentum; Brillouin zone; bandstructure; calculations with energy bands.

*Reading:* Foulkes, lecture 10

**2. Density-functional theory [2 sessions]**

**a. Theoretical concepts:** Schrodinger equation; Born-Oppenheimer approximation; Hellmann-Feynman theorem; variational principle; Hohenberg-Kohn theorems; Thomas-Fermi theory; The Levy approach; Kohn-Sham mapping; exchange and correlation functionals; properties of exact DFT; Janak's theorem; the derivative discontinuity and band-gap problem.

*Reading:* Martin, chapters 6 & 7 (excluding 6.4, 7.6 & 7.7)

**b. Practical calculations:** Finding the ground state; self-consistency; pseudopotentials; transferability; Brillouin zone integration; basis sets, with a focus on plane-waves.

*Reading:* Martin, chapters 12 & 13 (in particular 12.1, 12.2, 12.3, 12.7, 13.1)

**3. Wannier functions [2 sessions]**

**a. Theoretical concepts:** Wannier function for a single band and the concept of gauge freedom; Wannier functions for composite bands; criteria for choosing the gauge (including maximal-localization); exponential localization of Wannier functions in insulators; the case of entangled bands.

*Reading:* Marzari, sections II and III

**b. Applications:** analysis of chemical bonding; bandstructure interpolation and band derivatives; model Hamiltonians.

*Reading:* Marzari, sections IV, VI, VII

**4. Electronic excitations [3 sessions]**

**a.** Motivation from experiments involving electronic excitations.

*Reading:* Onida, chapter 1

**b.** Time-dependent DFT.

*Reading:* Zuehlsdorff, sections 4.1 & 4.2

**c.** Many-body perturbation theory, the GW method and the Bethe-Salpeter equation.

*Reading:* Zuehlsdorff, sections 4.3 & 4.4

**Key to references**

- **Foulkes:** WMC Foulkes, Electronic Structure of Materials lecture notes (2013-14)

- **Martin:** RM Martin, *Electronic Structure: basic theory and practical methods*
- **Marzari:** N Marzari, AA Mostofi, JR Yates, I Souza and D Vanderbilt, “Maximally localized Wannier functions: Theory and applications”, *Rev Mod Phys* **84**, 1419 (2012)
- **Onida:** G Onida, L Reining and A Rubio, “Electronic excitations: density-functional versus many-body Green’s-function approaches”, *Rev Mod Phys* **74**, 601 (2002)
- **Zuehlsdorff:** T Zuehlsdorff, PhD Thesis, “Computing optical properties of large systems” (Imperial College London, 2015)

#### **Optional light reading for the interested**

- R Jones, *Psi-k Highlight* 124 (2014)
- K Burke, *J Chem Phys* 136, 150901 (2012)
- G Ceder, *MRS Bulletin* 31 (2006)
- N Marzari, *MRS Bulletin* (2006)
- S Redner, *Physics Today* (2005)

#### **More advanced texts on DFT for the interested**

- Dreizler & Gross, *Density Functional Theory: An Approach to the Quantum Many-Body Problem*
- Fiolhais, Nogueira & Marques (Eds), *A Primer in Density Functional Theory*

# Classical Field Theory of Materials (CFTM2)

Dr Daniel Balint

8 hours of classes in Term 2

## Prerequisites:

- Mathematics for the Theory of Materials Parts 1 & 2
- Classical Field Theory of Materials Part 1

## Continuous assessment:

There will be three marked assignments covering the first three units of course material, as defined below, requiring the solution (and reporting of associated background and explanation) of one problem for each unit; the fourth unit, as defined below, is an available topic for the viva (in addition to the other three) but will not be assessed via a marked assignment. Feedback will be provided during the working of the solutions and preparation of the reports, and after the reports are marked.

## Examination:

- Viva voce examination

## Synopsis

1. Complex variable analysis of plane isotropic linear elasticity: stress functions; derivation of the biharmonic equation; conversion of the biharmonic equation into complex space for plane strain and plane stress; derivation of the equations for the stresses, displacements and force in terms of complex potentials; solution of a point (line) load and edge dislocation in an infinite elastic space.
2. The method of analytic continuation applied to complex variable analysis of plane isotropic linear elasticity; analytic continuation of a function from one domain to another; entire functions; derivation of useful identities for complex functions on boundaries between adjacent domains of analyticity; solution of a line load and dislocation in a half space; conformal mappings.
3. The distributed dislocation technique for modelling cracks; the analogy between dislocations and cracks under mode I, II and III loading; boundary conditions in terms of Burgers vector density; formulation of the integral equations; singularities and special polynomial expansions; numerical solutions techniques.
4. Plane discrete dislocation plasticity; the linear superposition principle; plane strain slip systems and slip system definition; Frank-Read and homogeneous nucleations; annihilations, pinning events; grain boundary descriptions; computational setup; capabilities and limitations; numerical issues, including time discretisation issues such as collisions, overtaking events and special cases, and resolution of the reduced boundary conditions

## Books

L E Malvern, *Introduction to the Mechanics of a Continuous Medium*, Prentice-Hall (1969).

N I Muskhelishvili, *Some Basic Problems in the Mathematical Theory of Elasticity*, Noordhoff (1977).

R W Soutas-Little, *Elasticity*, Dover (2012).

I S Sokolnikoff, *Mathematical Theory of Elasticity*, McGraw-Hill (1956).

J P Hirth and J Lothe, *Theory of dislocations*, Krieger (1992).

## Papers

R E Worden, L M Keer, *Green's functions for a point load and dislocation in an annular region*, Journal of Applied Mechanics 58 (1991), 954-959.

R G Stringfellow, L B Freund, *The effect of interfacial friction on the buckle-driven spontaneous delamination of a compressed thin film*, International Journal of Solids and Structures 30 (1993), 1379-1395.

D S Balint, J W Hutchinson, *Mode II Edge Delamination of Compressed Thin Films*, Journal of Applied Mechanics 68 (2001), 725-730.

F Erdogan, G D Gupta, *On the numerical solution of singular integral equations*, Quarterly of Applied Mathematics 29 (1972), 525-534.

E van der Giessen, A Needleman, *Discrete dislocation plasticity: a simple planar model*, Modelling and Simulation in Materials Science and Engineering 3 (1995), 689-735

# Computational methods (CMM)

## Matlab Primer [Computational Methods Hub]

Dr Prasun Ray

### One 4-hour computational lab in week 1 of Term 1

This course provides a quick, (hopefully) painless introduction to matlab for CDT students. It does not assume any prior matlab experience and should also be helpful to students who have used matlab in the past but would like a quick refresher. The course introduces students to the 'basics': using matlab for elementary linear algebra, programming, and data visualisation. This primer is intended to give students a head-start on their cohort challenge project in week 1 of Term 1.

#### Getting started

Students will need their CDT laptop with Matlab installed.

\*\*\*

## Introduction to HPC

*[Part of the Introduction to High Performance Scientific Computing course offered by the Computational Methods Hub]*

Dr Prasun Ray

### 10 hours of classes and 4 hours of computational labs in Term 1

This course is intended to bring students up to speed with working in a unix-/linux-based environment and introducing them software version control and programming in Python and Fortran. No previous experience is assumed.

**Lecture 1.** Course Overview. Getting started - working with UNIX and the command line

**Lecture 2.** Software version control with GIT and Bitbucket

**Lectures 3 – 6.** Programming and scientific computing with Python

**Lectures 7-10.** Introduction to Fortran 90 - modular programming and using popular libraries; interfacing with Python with F2Py

#### Assessment:

This section is worth 25% of the CMM grade.

There will be two assessed assignments.

For further details see <http://www.imperial.ac.uk/computational-methods/cm-hub/hpc-intro/>

\*\*\*

## Numerical Methods

Dr Éamonn Murray

### 10 hours of contact time in Term 1

This course gives students a solid practical background in numerical methods as used in day-to-day research in the theory and simulation of materials. Students must have taken the first half of the CM Hub course "Introduction to HPC" before this course.

#### Synopsis:

- With a focus on effective use of libraries and how these are used in scientific codes, this will cover the following topics: root finding, optimization problems, numerical integration, solving differential equations, solving systems of equations, Ewald summation, big data & machine learning techniques.

#### Course Material:

All course material will be freely available online at

<https://gitlab.com/eamonn.murray/NumericalMethods>.

### Recommended Reading:

- Christian Hill, *Learning Scientific Programming with Python*, Cambridge University Press (2016).

### Assessment:

This section is worth 25% of the CMM grade.  
There will be four marked assignments.

### Plagiarism policy:

In this course, students are welcome to collaborate and compare results, and are encouraged to do so to cross-check their codes and identify bugs, but **every student must write and comment their own code**. Where students have used some code they've obtained from elsewhere, it must be referenced clearly in the comments. Students who don't write their own code where asked, won't really get anything out of this course.

\*\*\*

## Group Programming Project

Dr Éamonn Murray

### 8 hours of contact time in Term 2

The ability to develop software collaboratively in an effective way, using modern tools is extremely valuable skill. Scientific computing tools are most often written by groups of researchers working together, and this is also true for any other software package. This course will give students direct experience of this process, by working together in groups to develop a useful piece of software.

The cohort will be divided into several groups and given a set of minimum requirements for a piece of software to solve a scientific problem. They will work together using a git repository to develop their code which will be due on the first day of reading week in Term 2.

Students will be responsible for setting their own goals and workload distribution. In addition to weekly consultations with the course coordinator, flexible office hours will be available.

### Assessment:

This section is worth 50% of the CMM grade.

Each group's final code will be graded according to the following criteria:

- Clarity (25%): How easy is it to understand the final code structure as written and how well documented is the code?
- Function (25%): Does the code work correctly and how easy is it to use? Does the code do more than the minimum?
- Effective collaborative development (25%): How effectively was the project divided into smaller tasks and these divided between group members, as evidenced in the git log for the project?
- Speed & Scaling (5%): How fast is the final code and how well does it scale with problem size?
- Student peer-to-peer allocation (20%): A proportion of the marks for this option is left for the members of the group to distribute among themselves, providing an opportunity for further practical experience of the interpersonal skills involved in collaborative work (e.g., negotiation, communication and etiquette). Students may allocate marks to individual members of the group according to the level and impact of individual contributions. The total number of marks available in this category is determined by the score obtained in the other categories. When deciding the distribution of marks, students are encouraged to think about how each member of the team has
  - ☐ Contributed to structuring the work and deciding on the code structure and division of tasks;
  - ☐ Contributed to the writing and testing of the code;
  - ☐ Helped and supported other members of the team throughout the project.

# Group project



## Group Research Strategy Project (GRSP)

Dr Arash Mostofi

### 10 hours of contact time in Term 2

When confronted with a complex challenge, the ability to logically analyse and break it down into manageable parts is one of the most important skills, whatever your chosen profession.

In the specific context of scientific and technological challenges, this means: (i) researching and understanding the background to the problem and the wider context in which it sits; (ii) deconstructing the problem into a hierarchy of hypotheses and questions that are each more easily amenable to scientific investigation than the broader challenge itself; (iii) designing a programme of research to test these hypotheses and questions; (iv) articulating the strategy in a scientifically sound and coherent manner and, importantly, (v) doing so a persuasive manner so that the importance and impact of the work is clear to a potential funder.

Having a good all-round knowledge of materials is an advantage, but the ability to get to the heart of a complex problem and develop a strategy to solve it is the essence of a successful research scientist. The objective of the *Group Research Strategy Project* (GRSP) is to enable students to experience this process, from being presented with a materials-related challenge, all the way through to writing a research proposal on how to tackle it using theory and simulation. Students will work together in groups, thereby providing direct experience of collaboration and teamwork, which are essential in modern scientific research. Note that the GRSP does not require students to solve the problem presented itself, but to develop the research strategy for doing so.

The specific problem will be suggested by one or more industrial partners of the CDT. Each group will liaise with the industrial partner to understand the problem in detail. Each group will then work towards developing a research proposal, in the style of an EPSRC Standard Grant application.

Proposals will be evaluated according to the same criteria as EPSRC Standard Grants, namely: the clarity and excellence of the proposed research and appropriateness of the methodology proposed; the importance and impact of the work; and the appropriateness of the planning and management of resources requested.

The deadline for research proposals is **Friday 22<sup>nd</sup> March 2019 at 5pm**. Proposals should be emailed by the deadline as a single PDF document to Arash Mostofi and Miranda Smith.

The course is intended to be student-led and the students will be responsible for most aspects of the course, including setting their own goals, deadlines, and workload distribution. In addition to a weekly meeting with the member(s) of academic staff running the course, flexible office hours will be available. Organising and chairing the meetings will be a responsibility of the students.

There will be a meeting to discuss the course towards the end of Term 1.

### Assessment

#### *Written proposal (40%)*

Each group's proposal will be reviewed by at least two reviewers and according to EPSRC's review criteria and slightly modified for the purposes of GRSP.

#### *Panel interview (20%)*

Each group will receive their anonymous reviewer reports a few days in advance of their panel interview, which will be held in Term 3 at a date to be determined. At the panel interview, each group will have the opportunity to give a 10 minute presentation about their proposal (A/V facilities will be available if required), which will be followed by up to 30 minutes of questions and discussion. In addition to exploring aspects of the proposal in more detail, the interview provides the research team the opportunity to respond to comments in the reviewer reports.

#### *Student peer-to-peer allocation (40%)*

A proportion of the marks for this option is left for the members of the group to distribute among themselves, providing an opportunity for further practical experience of the interpersonal skills involved in collaborative work (e.g., negotiation, communication and etiquette). Students may allocate marks to individual members of the research team according to the level and impact of individual contributions. The total number of marks available in this category is determined by the average obtained in the written proposal and panel interview. When deciding the distribution of marks, students are encouraged to think about how each member of the team has:

1. Contributed to the thinking in the proposal;
2. Contributed to the writing of the proposal;
3. Helped and supported other members of the team throughout the project;
4. Contributed to the planning and preparation for the interview.

### **EPSRC standard proposal structure**

Standard EPSRC proposals have the following general structure, to which your proposal must adhere. Proposals must be on A4 paper, in Arial font (minimum size 11pt), with margins no less than 2 cm on all sides. The page limits specified below must be strictly adhered to.

- Case for Support (up to 6 pages), covering (not necessarily in this order):
  - Background
  - National Importance
  - Academic Impact
  - Research Objectives
  - Programme and Methodology
  - Timeliness
  - Risk
  - Resources and Management
- Justification of Resources (up to 2 pages)
- Workplan (up to 1 page)
- Pathways to Impact (up to 2 pages), including (not necessarily in this order):
  - Society: quality of life, policy, international development, health
  - Knowledge: scientific advances, techniques
  - People: skills
  - Economy: wealth creation, new products, new companies, inward investment

Note that the 2-page section on “Track Record” of the applicants, present in the standard EPSRC proposal structure, is not required for the purposes of GRSP, nor are CVs of named collaborators or Letters of Support.

Further resources that will be helpful when writing your proposal:

- EPSRC guidance on preparing a proposal (including advice on National Importance and Impact):
  - <http://www.epsrc.ac.uk/funding/howtoapply/preparing/>
  - <http://www.epsrc.ac.uk/funding/howtoapply/preparing/includingnationalimportance/>
  - <http://www.epsrc.ac.uk/funding/howtoapply/preparing/economicimpact/>
- EPSRC guidance on Pathways to Impact
  - <https://epsrc.ukri.org/innovation/fundingforimpact/pathwaystoimpact/>
- EPSRC (challenge) themes:
  - <http://www.epsrc.ac.uk/research/ourportfolio/themes/>
- The EPSRC portfolio:
  - <http://www.epsrc.ac.uk/research/ourportfolio/>
  - <https://www.epsrc.ac.uk/funding/howtoapply/preparing/writing/>

## GRSP Assessment criteria

Your proposal and interview will be assessed according to EPSRC's Standard Grant Review Criteria, modified accordingly for GRSP:

1. Quality
  - a. Novelty, context, timeliness
  - b. Ambition, transformative aspects
  - c. Methodology
2. Importance
  - a. National importance on 10-50 year timeframe in relation to other research in the area
  - b. How research contributes to: other research areas; societal challenges and EPSRC challenge themes; UK economy; emerging industry
3. Impact
  - a. How complete and realistic are the impacts identified?
  - b. Effectiveness of activities identified to realise impacts
  - c. Relevance of beneficiaries and collaborators
4. Resources and Management
  - a. Appropriateness of resources requested
  - b. Viability of management plans (eg, access to equipment, third-party contributions)

## Appendix 2 Guidelines for the Conduct and Assessment of Research Projects

### Introduction

The research project is the single most important (in terms of its contribution to your final mark), and probably the most enjoyable, component of your MSc degree. Including the literature review, it counts for 40% of your overall MSc. The assessment of the literature review accounts for 25% of these marks, the research project report forms 60% of the marks available, and the assessment of the research project presentation the remaining 15%.

### The Literature Review

Starting after the conclusion of the oral examinations at the end of Term 2, you will work on a literature review of the topic of your research project. Your supervisor will give you some suggested reading to get you started and a title for your review to give it a focus. A good literature review not only summarises what has been written about a particular topic (with comprehensive references), but compares and contrasts differing results, analyses and theories, providing a critical commentary on recent work in the field. Your literature review will take the form of a written report, **not exceeding 3,000 words in length** (including captions to figures and tables, but excluding any cover page, table of contents, acknowledgements, references and appendices). It will be assessed both on scientific quality and its presentation and readability. The deadline for this is **5pm on Friday 10<sup>th</sup> May 2019**. The literature review will be assessed by your supervisor, who will provide feedback that should help you with your main research project report. A declaration of the word count must be included on the first or cover page of the literature review.

### The Research Project Plan

The research element of your project starts after you submit your literature review. By the end of the first month of your project, you should write a short (one side A4 maximum) plan that gives:

1. a concise summary of the motivation for your project and its multiscale aspects;
2. a short project plan, stating clearly each aim and objective, and how and when you expect to achieve each one.

You should then arrange to meet with your supervisors before **Friday 14<sup>th</sup> June 2019** to discuss your plan. The plan is not assessed, but it is important that it is used as an opportunity to be candid and honest so that potential problems may be identified. The template for the research plan may be found at the end of this document.

### The Research Project Presentation

The project presentations will take place on **Friday 30<sup>th</sup> August 2019**, as part of the MSc Conference. You will be required to give a 10-minute presentation, followed by 5 minutes of questions and discussion. Your performance will be assessed by a panel of academic staff. Assessment of the project presentation will include how well you present your work in an engaging, clear and informative way and handle the discussion and questions after your presentation. The assessment form is included for information at the end of this document.

### The Research Project Report

The report must be typeset using, e.g., Microsoft Word or LaTeX, and must not exceed **5,000 words** in length (including captions to figures and tables, but excluding the cover page, table of contents, acknowledgements, references and appendices). It will be assessed both on scientific quality and its presentation and readability. **You must submit an electronic version of your report in PDF format to the CDT Senior Administrator by 5pm on Friday 6<sup>th</sup> September 2019.**

## Report Structure

Try to be concise, yet complete, and to adhere in broad terms to the following structure, making allowances for the nature of your particular project:

Cover page. Include a title that clearly identifies what the report is about, the name of the author, the date of submission, and a formal statement as follows:

*“A thesis submitted in partial fulfilment of the requirements for the degree of Master of Science of Imperial College London.”*

A declaration of the word count must also be included.

An abstract that clearly and concisely identifies the principal features of the work, its multiscale nature, and the key results achieved (including numerical results where appropriate) and the conclusions that can be drawn, if any.

Content page(s), listing the chapters, sections, and subsections.

A formal acknowledgement section referring to the people you wish to thank. You should also clearly identify where in your project work you have received practical help and technical support from others. For example use of a pre-existing computer code, or work conducted as part of a team, etc.

An introductory chapter in which the broad aims and objectives of the project are established, the multiscale nature of the project is set out, and in which the work is clearly put into context with respect to existing work and previous literature.

Discussion of the methods employed. The methods may be computational and/or theoretical as appropriate to the project.

A clear description and presentation of the results/observations obtained. Think carefully about how to convey the results with clarity and in the most informative way. Data plots etc., which should always be referred to as figures, must have clearly labelled axes and scales and an extensive figure caption that states what is plotted and draws attention to the key points.

A critical discussion of the results, limitations and errors, and the conclusions that may be drawn from the results.

In your conclusions you should discuss the extent to which the aims of the project have been achieved and what further work would be appropriate. You should also identify clearly what your part in the work has been and acknowledge the work of others.

You must provide a clear and extensive set of references (bibliography) to which you have referred in the text. These should be in any one of the standard formats as used in scientific journals.

Lengthy mathematical derivations, computational algorithms and programs, and large quantities of data that you wish to place on record should be included as appendices and do not count towards the word limit.

It is most important that an experienced scientist should be able to read through the report and immediately be able to follow in detail what was done, to put the work into context and, in principle, be able to reproduce the project. If the project is computational, for example, exactly how the computation was approached should be described.

It must be stressed that reports must be complete and concise, and waffle must be avoided and all points made should be substantiated.

It is important to realise that most projects are never finished and the report should reflect what has been done within the limited time available. It is advisable, therefore, to plan well so as to have

achieved something by the time it comes to write up. In some cases it may seem that little has been achieved; this is no reason, however, for not producing an excellent report.

### **Assessment of the Report**

The project report will be marked by two independent assessors, who will be informed by a report from your supervisor, and your final mark will be an aggregate of the two. In the event that the two markers disagree by a significant margin, they will confer to arrive at a consensus mark. It may also be read and moderated by one or more members of the Board of Examiners. The assessment guidelines and assessment forms are included at the end of this document.

### **A Note on Plagiarism**

Plagiarism is illegal. The penalties are severe and may include expulsion from the College. Therefore, never use the words or ideas of others from any source, e.g. published papers, the web or other student reports, without a proper attribution. For further information, see the following websites:

<http://www.imperial.ac.uk/student-records-and-data/for-current-students/undergraduate-and-taught-postgraduate/exams-assessments-and-regulations/plagiarism-academic-integrity--exam-offences/>

The electronic submission of your report may be run through software to check for plagiarism.

**Please ensure that in each section of your report you state explicitly what is your own original work, what your supervisors contributed and what material is based on the literature.**

### **Working in an interdisciplinary research environment**

You will have more than one supervisor, but your principal supervisor will have overall responsibility for your project. You should have regular meetings with all your supervisors and you should discuss what you are doing and seek their feedback and guidance. It is quite possible that you will have to meet them separately because they are busy people. It is also quite possible that you may get conflicting advice! Don't be worried about such conflicts – they are not uncommon in an interdisciplinary environment, and indeed they can contribute to creativity and new ways of thinking. Be open with your supervisors about any conflicts that you detect in their advice, and try to resolve them with your supervisors. If you feel you need help talk to your Cohort Mentor. If the Cohort Mentor is unavailable contact the MSc Director or the Director of the CDT. These people will help you if you ask, but don't leave things too long before asking them.

- Don't be afraid to tell your supervisors that you don't know something or that you are stuck. They are there to help guide the project and need to know how things are progressing in a clear and honest manner.
- If you don't understand something, just keep asking questions until you do. The smartest people often ask the "dumbest" questions.
- Find out where and when the research groups of your supervisors have coffee, lunch, Friday evening drinks etc. and go along as often as possible. This is where lots of problems get solved through informal discussions and the occasional back-of-the-envelope calculation.
- Keep a complete and detailed "lab book" and bring it to every meeting you attend. Your lab book will be invaluable when you write up your final report.
- Some research groups have regular progress and planning meetings. If you are asked to attend, be on time and be prepared to explain what you have done, what you plan to do next, and justify any resources you need for the next stage of your project. Take up-to-date results and your lab book with you.
- Keep backups of all your results. Keep multiple backups! Hard disk space and USB memory are both cheap, so make sure that you cannot lose your data accidentally.
- As you are writing your report keep multiple backups. If your computer crashes you will not be given an extension of the deadline for submission of your report.
- If your project needs something to progress (equipment, software, computer time etc.) prepare a realistic plan and/or budget and present this to your principal supervisor.

## Expectations for MSc research projects

The TSM-CDT's expectations for the conduct of MSc research projects mirror the College's expectations for research project supervision (<https://www.imperial.ac.uk/study/pg/graduate-school/quality-assurance/phd-students-and-supervisors/>)

Supervisors can expect students to:

1. Take responsibility for your project. In the end it is your work and your supervisors are here to help you accomplish your research objectives, but not to do the thinking for you. This includes reminding your supervisors of upcoming deadlines and milestones.
2. Work hard. Imperial is a top-ranking University and we expect that students will strive to accomplish excellent work.
3. Display initiative. The person who drives the research is you. We expect you to be curious about your work and to think about how it connects with ideas in other fields of science. In light of this, it is a requirement for you to attend all planned supervisor meetings, group meetings, and other seminars offered by departments and/or the Thomas Young Centre.
4. Be critical of your own work and results, and use these skills in analyzing and evaluating results in the literature.
5. Help colleagues in your group to learn through discussions and demonstrations.
6. Keep up with the literature in your field.
7. Provide regular reports detailing your results. You should be conscientious about keeping a record of your work as this will make writing your final report much easier.

Students can expect supervisors to:

1. Be supportive, both intellectually and personally.
2. Set up a viable project and ensure that there are clear aims and objectives and an initial work-plan
3. Meet once a week for one hour to provide guidance and advice.
4. Be available (or provide an identified substitute) to talk about research problems at relatively short notice although a few days' notice may be needed.
5. Help develop independence and confidence in research skills.
6. Help develop skills in technical writing, oral presentations, problem solving, data analysis and critical literature reviews.
7. Read your literature review and project report thoroughly and make constructive comments on both style and intellectual content.

## Research Project Plan

**Student:**

**Project Title:**

**Supervisors:**

### **Project Outline and Plan.**

Please state the objectives of your project and when and how you expect them to be achieved.

**Student's signature:**

**Date:**



**Student:**

**Comments:** Please give written feedback on the student's project plan.

**Principal Supervisor's signature:**

**Date:**

**PLEASE COMPLETE AND RETURN TO CDT ADMINISTRATION OFFICE**  
**Page 2/2**

## Literature Review and Research Project Report Assessment Guidelines

**The marking scheme uses the criteria below.** It might very well be that different aspects of the report fall into different marking bands. For example, the student may give a very good account of the background material and relevant literature, but the report shows little understanding, or vice versa. In such cases, please use your discretion to assign the mark.

- 90 – 100 %** Exceptional high quality work that clearly demonstrates a substantial independent contribution and originality at research level in addition to a thorough understanding of the topic. Comprehensive and authoritative discussion of background material and relevant literature is included. The work is of a quality that with little effort is publishable on its own or as part of an article in a peer-reviewed journal.
- 80 – 90 %** Very high quality work that clearly demonstrates independent contributions and originality at research level in addition to an authoritative account of the work undertaken with almost no gaps in the understanding of the topic. A comprehensive discussion of background material and discussion of relevant literature is included. The work is of a quality that, with some effort, is publishable as part of an article in a peer-reviewed journal.
- 70 – 80 %** Very good work demonstrating an authoritative account with relevant material throughout and with independent contributions by the student. There are only minor gaps in the understanding of the project work. A very good discussion of background material and relevant literature is included. Some of the work is of a quality that it could contribute to aspects of a publishable article in a peer-reviewed journal.
- 60 – 70 %** Good work with relevant material and authoritative in most places, including some independent contributions by the student. Only a few gaps and few deficiencies in the discussion and understanding in minor parts of the report. A good discussion of background material and relevant literature is included.
- 50 – 60 %** Satisfactory with relevant material in most places and possibly authoritative in some places. Some gaps and some deficiencies in the discussion and understanding in some parts of the report. Some background material and discussion of relevant literature is included.
- 40 – 50 %** Adequate with relevant material in some places. Large gaps and large deficiencies in the discussion and understanding in various parts of the project. Adequate discussion of background material and relevant literature is included.
- 30 – 40 %** Unsatisfactory but with some relevant material in some places. Of some merit but considerable gaps and considerable deficiencies in the discussion and understanding in major parts of the project. Little discussion of background material and/or relevant literature is included.
- 15 – 30 %** Very unsatisfactory with only small amount of relevant material. Of little merit with substantial gaps and substantial deficiencies in the discussion and understanding in major parts of the project. Almost no discussion of background material or relevant literature is included.
- 0 – 15 %** Highly unsatisfactory with almost no relevant material anywhere. Of no or very little merit. No discussion of background material or relevant literature is included.

## Assessment of the literature review by the principal supervisor

**Student:**

### 1. Coverage of the Review

Mark out of 25 the extent to which the student has identified the literature relevant to the title of the review and selected pertinent issues to focus on in the review.

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

### 2. Understanding of the Subject

Mark out of 25 for the degree of understanding shown of the literature reviewed, both of the theoretical concepts and simulation methods described.

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

### 3. Critical Thinking

Mark out of 25 the degree of critical thinking demonstrated by the student, including the identification of conflicting points of view, weighing of the evidence on each side, judgment shown and the identification of future work required.

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

### 4. Presentation of the Review

Mark out of 25 for the logical structure and presentation of the work, the extent to which the English is grammatical and accurate, and the quality of any figures and graphs. Consider also the overall usefulness of the review as a scientific document.

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

**TOTAL MARK:**

**out of 100.**

**Student:**

**Comments.** Please give written feedback to justify the marks awarded. These written comments (which need not be typed) will be passed on to the student. Please highlight the aspects that the student did well and provide constructive criticism and advice on how to improve.

**Name of principal supervisor:**

**Signature:**

**Date:**

**PLEASE COMPLETE AND RETURN TO CDT ADMINISTRATION OFFICE**

**Page 2/2**

**Report on the research project by the principal supervisor**

**Student:**

**External factors:**

Please comment on the circumstances and environment that the student experienced during the research project. This should include a description of the extent of help received from other members of your research group or the provision of simulation software to use. Please also mention any circumstances outside the student's control that may have adversely affected their execution of the project e.g. unavailability of resources, staff absence or a bug in a code supplied to the student.

**Student performance:**

Please comment on the student's performance in executing the research project, including the extent of their achievements and the level of skill in carrying out the project. This might include skills in computing, theory, novelty in bridging length or time scales, etc. – whatever is appropriate for the individual project.

**Principal Supervisor's signature:**

**Date:**

**PLEASE COMPLETE AND RETURN TO CDT ADMINISTRATION OFFICE**

**Page 1/1**

## Assessment of the research project report by an independent assessor

**Student:**

### 1. Scientific Background

Basing your judgement on the content of the report alone give a mark out of 25 for the understanding shown of the scientific background of the project, the multiscale aspects related to the project, and the motivation for the project.

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

### 2. Understanding Demonstrated by the Report

Mark out of 25 for the level of understanding demonstrated by the student in the report, including the presentation of the results and their analysis, the justification of the conclusions reached, and the identification of further work.

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

### 3. Student Achievement and Use of Skills

Basing your judgement on the contents of the student's and supervisor's reports give a mark out of 25 for the level of achievement and skill shown by the student. This might include skills in computing, theory, novelty in bridging length or time scales, etc. – whatever is appropriate for the individual project.

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

### 4. Presentation of the Report

Mark out of 25 for the logical structure and presentation of the work, the extent to which the English is grammatical and accurate, and the quality of the figures and graphs. Consider also the overall usefulness of the report as a scientific document.

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

**TOTAL MARK:** \_\_\_\_\_ **out of 100.**

**Student:**

**Comments.** Please give written feedback to justify the marks awarded. These written comments (which need not be typed) will be passed on to the student. Please highlight the aspects that the student did well and provide constructive criticism and advice on how to improve.

**Name of assessor:**

**Signature:**

**Date:**

**PLEASE COMPLETE AND RETURN TO CDT ADMINISTRATION OFFICE**  
**Page 2/2**

Research Project Presentation Assessment Form

Student:

Did the student:

[a] explain how the work fitted into the context of related work?

0 1 2 3 4 5 6 7 8 9 10

[b] give a clear summary of the work undertaken and of the multiscale aspects of the project?

0 1 2 3 4 5 6 7 8 9 10

[c] present clearly the scientific conclusions that could be drawn?

0 1 2 3 4 5 6 7 8 9 10

[d] give a logically structured and interesting presentation with legible and informative slides?

0 1 2 3 4 5 6 7 8 9 10

[e] express themselves clearly and audibly during the presentation, and field the questions well?

0 1 2 3 4 5 6 7 8 9 10

TOTAL MARK: \_\_\_\_\_ out of 50.

**Comments:** Please give written feedback to justify the marks awarded. These written comments (which need not be typed) will be passed on to the student. Please highlight the aspects that the student did well and provide constructive criticism and advice on how to improve.

Assessor's name:

Signature:

Date:

PLEASE COMPLETE AND RETURN TO CDT ADMINISTRATION OFFICE