



Trinity College Dublin

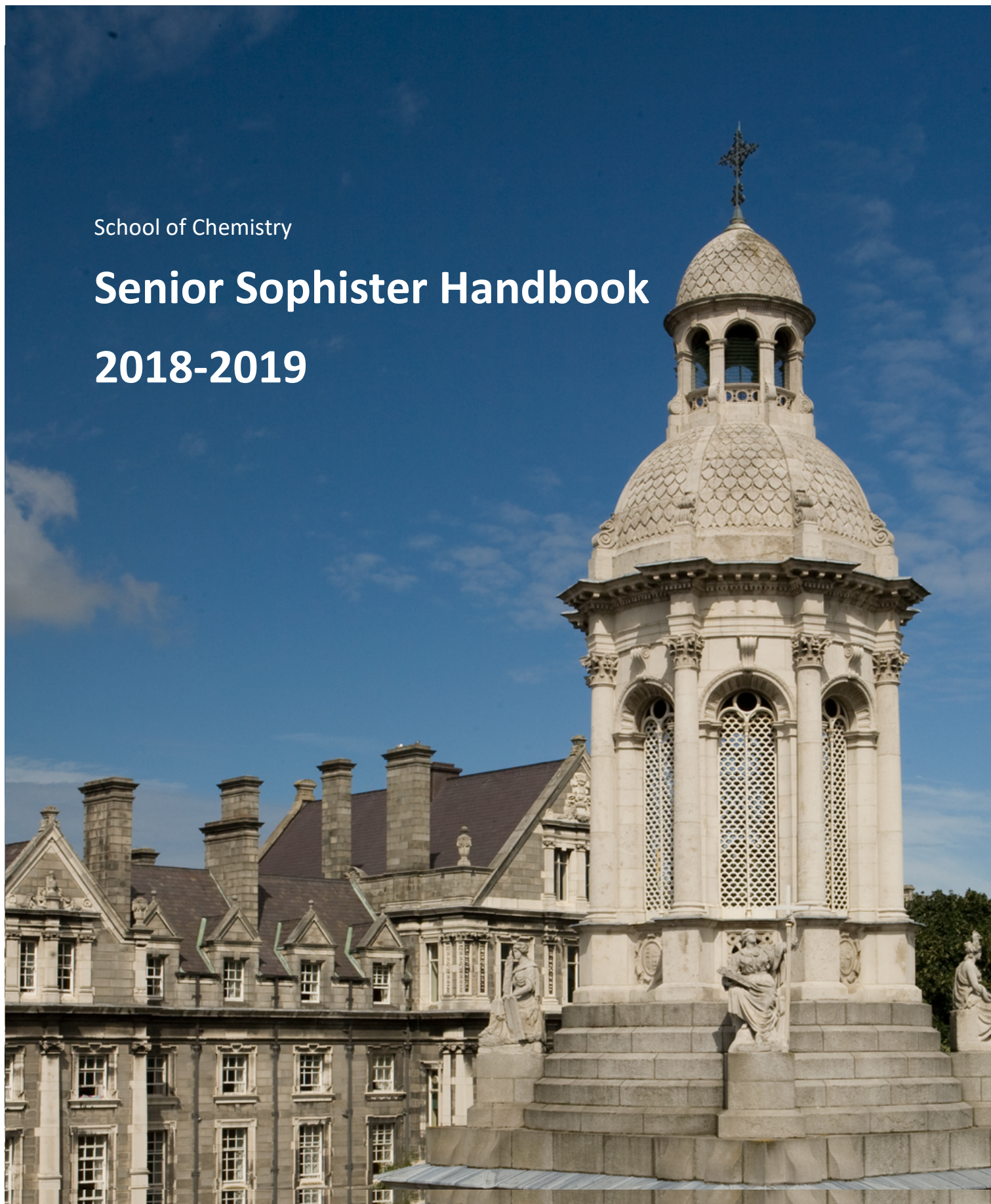
Coláiste na Tríonóide, Baile Átha Cliath

The University of Dublin

School of Chemistry

Senior Sophister Handbook

2018-2019



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Alternative formats of this Handbook can be made available upon request. A large-print hard copy is also available to view in the School Office.

Information for all School of Chemistry SS Students

Senior Sophister 2018/19

Welcome to your final year of undergraduate study in Trinity. Prof. Valeria Nicolosi (Senior Sophister Coordinator), Prof. Mathias Senge (Course Director of Medicinal Chemistry), Prof. Graeme Watson (Course Director of Chemistry with Molecular Modelling) and Profs. Paula Colavita and Eoin Scanlan [Director and Associate Director of Teaching and Learning (Undergraduate), respectively] will liaise with you during the year, will be available to discuss any problems that may arise, and to give you all the advice and help that they can. Other members of staff, of course, will also be happy to talk with you and to discuss any problems that may arise. The details of your course for the year are set out in this handbook, together with information about your final examinations. As the N-PCAM course is shared between the Schools of Physics and Chemistry, it has a separate course structure to the School's other moderatorship degrees. At present (2017/18–2019/20), the School of Physics is responsible for administration of the N-PCAM programme and will provide information on the dedicated nanoscience website at <http://www.tcd.ie/nanoscience/>. The N-PCAM Course Director is Prof. Hongzhou Zhang, School of Physics.

Course-specific webpages

Each course offered by the School has a dedicated webpage. For those in N-PCAM, there is also a dedicated nanoscience website at <http://www.tcd.ie/nanoscience/>.

http://chemistry.tcd.ie/Study/current_students/undergraduate/chemistry/ss/index.php

http://chemistry.tcd.ie/Study/current_students/undergraduate/medicinal-chemistry/ss/

http://chemistry.tcd.ie/Study/current_students/undergraduate/CMM/ss/

and

http://chemistry.tcd.ie/Study/current_students/undergraduate/N-PCAM/index.php

Emergency Procedure

In the event of an emergency, dial Security Services on extension **1999**.

Security Services provide a 24-hour service to the college community, 365 days a year. They are the liaison to the Fire, Garda and Ambulance services and all staff and students are advised to always telephone extension 1999 (+353 1 896 1999) in case of an emergency.

Should you require any emergency or rescue services on campus, you must contact Security Services. This includes chemical spills, personal injury or first aid assistance. It is recommended that all students save at least one ICE (in case of emergency) phone number in their mobile phones.

Contact Details

Position	Person	E-mail	Phone
Head of School	Prof. Mike Lyons	melyons@tcd.ie	896 1423
Director of Teaching and Learning (DTLUG)	Prof. Paula Colavita	colavitp@tcd.ie	896 3562
Associate DTLUG	Prof. Eoin Scanlan	scanlae@tcd.ie	896 2514
SS Year Coordinator	Prof. Valeria Nicolosi	nicolov@tcd.ie	896 4408
MedChem Director	Prof. Mathias Senge	sengem@tcd.ie	896 8537
CMM Director	Prof. Graeme Watson	watsong@tcd.ie	896 1357
N-PCAM Director	Prof. Hongzhou Zhang	Hongzhou.Zhang@tcd.ie	896 4655
School Manager	Dr. Sinéad Boyce	sboyce@tcd.ie	896 4587
School Office	Ms. AnneMarie Farrell	farrea25@tcd.ie	896 1726
School Office	Ms. Jennifer McHugh	mchughj7@tcd.ie	896 2040
Global Officer	Dr. Niamh McGoldrick	nmcgoldr@tcd.ie	896 3463

Contact details for all staff in the School can be found at <http://chemistry.tcd.ie/staff/>

Staff, Research and Facilities

The School currently has 25 academic staff and 14 technical staff. The School has an active research programme, with approximately 130 postgraduate students and postdoctoral researchers. They study a wide range of chemistry subjects in fields such as organic, inorganic, organometallic, physical, theoretical, medicinal, analytical, material, polymer, environmental, and supramolecular chemistry. Research income is earned from national, international and commercial sources and the School has held grants in all relevant research programmes funded by the EU.

The College also fosters an interdisciplinary approach to research, with members of the School having strong links with colleagues in the physical, medical, technological and biological sciences both within College, nationally and internationally.

The School is well equipped for its research activities, having Bruker 600 and 400 MHz and access to an Agilent 400 MHz high-field multi-nuclear NMR, FTIR, dispersive IR and UV-Vis spectrometers, high performance liquid chromatography (HPLC) and gas chromatography (GC) equipment, a Bruker SMART Apex Kappa Duo, Bruker D8 Quest ECO single crystal and a Bruker D2 Phaser powder diffractometer, a Micromass LCTM (TOF) mass spectrometer, thermogravimetric analysis and differential scanning calorimetry, dynamic light scattering, several spectrofluorimeters for steady-state and time-resolved fluorescence measurements, circular and linear dichroism, and a large range of wave generators and potentiostats for cyclic voltammetry.

Lectures

Lectures should begin on the hour and end 50 minutes later. Timetables will be published through the portal <https://my.tcd.ie> and should be checked regularly for changes to the original schedule. Module descriptors and learning outcomes for your modules are available on Blackboard. Details related to fees, assessment, exam timetables etc. can be found on the Academic Registry's website at <https://www.tcd.ie/academicregistry/>.

Capstone Project

You will carry out your capstone project in Semester 1. For those working in the School of Chemistry, the project will be carried out under the supervision of a member of staff and must

be completed by the end of the semester. **Project work will begin in Trinity College on Monday 10 September 2018 and a compulsory safety workshop has been organized for Tuesday 11 September 2018.**

ERASMUS and other projects carried out abroad start approximately two weeks earlier (27 August) than the start date in Trinity. Students who opt to do their project abroad will normally be allocated a “home mentor”, i.e. a member of the academic staff in the School who will act as a contact with the student while they are away and will be available to give advice and assistance. Students who have queries or encounter problems should contact their home mentor as soon as possible. In the absence of a home mentor, students should e-mail the International Coordinator ([Prof. Dunne](#)), cc’ing the SS Year Coordinator ([Prof. Nicolosi](#)) and the DTLUG ([Prof. Colavita](#)).

All students must submit their final project report electronically **no later than 16:30 on Friday 30 November 2018**. In an attempt to create a fair evaluation method and to keep in line with College guidelines on plagiarism, the software “TurnItIn” will be used for electronic report submission. Details and guidance on how to use this software will be sent to you later in the year. Two hard copies of the identical report to that submitted electronically should be handed in to the School Office **no later than 16:30 on Monday 3 December 2018**.

You should discuss the structure and content of your report with your supervisor. **It must be typed using a font size of 12, and be double-spaced, bound, and no more than 30 pages in length.** In addition to this page limit, you can include limited numbers of spectra *etc.* as an appendix. Your laboratory notebooks, together with appendices of spectra *etc.* must also be handed in at this time. It is crucial that you allow sufficient time for the completion of your report. Your supervisor must receive a draft copy of your report **by Friday 16 November 2018**. Two formal meetings will be held with Senior Sophisters to discuss work progress and the writing of the report during the first semester (dates to be set). Those of you opting to carry out your project abroad will receive this information from your home mentor/SS Coordinator. The presentation slides given to students remaining in TCD will be uploaded to the SS course pages, e.g. http://chemistry.tcd.ie/Study/current_students/undergraduate/chemistry/ss/index.php

Project Assessment: Marks for your project contribute 33.33% to your SS year mark and will be allotted based on quality of content, presentation, effort made and performance during the project work, thesis preparation and oral examination. The outlined assessment structure will apply to all except N-PCAM students, both those doing projects in TCD and those doing projects abroad. Your project work will be assessed by three academics, one of whom will be your supervisor. The supervisor will submit a written report on the work conducted during the project and will contribute to 20% of the project marks. The other two assessors will assess the project report and conduct a formal assessment that will each contribute to 40% of your overall mark. The assessment will involve a 10- minute presentation by the student followed by a question and answer session in which the work and underlying theoretical concepts will be discussed. If there are significant mark discrepancies between the project assessors, the Director of Teaching and Learning (Undergraduate), Prof. Colavita, may appoint adjudicative assessors to ensure a balanced and fair evaluation of the written report. Oral examinations will be scheduled between **Monday 10 December and Friday 14 December 2018**. Your supervisor will have no role in these oral examinations.

Problem Solving Assessment: In addition to discussing the project, the oral assessment will also include a separate examination of the problem-solving element of the option and problem-solving module (CHU44108/CHU44408/CHU44708). The outcome of this part of the oral assessment will contribute to 10% of the total module mark.

If you have further queries about the research project contact Prof. Valeria Nicolosi (nicolov@tcd.ie) or the School of Chemistry Office, either in person or by e-mail to AnneMarie Farrell at farrea25@tcd.ie.

Summary of dates associated with your capstone project

Approx. 27 August	Projects abroad start
10-September	Projects start at TCD
11-September	Safety workshop
30-October	Deadline for submission of solutions in hardcopy to the 6 problems in the problem assignment
16-November	Draft of project report to supervisor
30-November	Submission deadline for electronic copies of project reports
03-December	Submission deadline for hard copies of project reports to School Office
10–14 December	Project presentations and oral examinations

Examinations

An overall pass mark of 40% is required to pass the Senior Sophister year. Full details of the Science (TR071) examination regulations may be found in the Appendices. The same regulations apply to the School's direct-entry courses. Past examination papers are available from the Academic Registry's website (<https://www.tcd.ie/academicregistry/exams/past-papers/annual/>) and can be used to familiarize yourself with the structure of examination papers, although you should bear in mind that some modules have been combined into 10-ECTS modules to comply with the introduction of the TEP programme in 2018/19. You will be given clear instructions on how this change impacts the exam structure later in the year. Your JS Chemistry mark contributes to **35%** of your final Moderatorship degree mark. Further information can be found in Appendix 1.

Feedback and Evaluation

The courses offered by the School benefit from student feedback. Rather than waiting until the end of a module to request online feedback, the School of Chemistry has instituted a Sophister Liaison Committee (SLC). Committee members comprise the DTLUG/Associate DTLUG, the School Convenor, JS and SS class reps, and Heads of Discipline or their representatives, and the meetings are minuted. Class reps should collate feedback from their fellow students to bring to the meetings, which takes place at least once per semester.

Academic Year Structure

Academic Year Structure 2018/19

Key Dates

SS Induction	Monday 10 September 2018
SS Safety Workshop	Tuesday 11 September 2018
Study/Review Weeks:	Monday 22 October to Friday 26 October 2018
Revision Week Semester 1:	Monday 3 December to Friday 7 December 2018
Study/Review Week:	Monday 4 March to Friday 8 March 2019
Revision Week Semester 2:	Monday 15 April to Friday 19 April 2019
Trinity week:	Monday 29 April to Friday 3 May 2019
Formal Assessment weeks	
Semester 1 examinations	Saturday 8 December to Friday 14 December 2018
Semester 2 examinations	Tuesday 23 April to Saturday 27 April 2019 (and Tuesday 30 April and Thursday 2 May 2019 if required)

Seminars and Special Lectures

You are expected to attend the School's research seminars, which are held at noon on Thursdays during both semesters. Talks will be advertised on the School website at <http://chemistry.tcd.ie/>. During the year, lectures on various topics will be arranged by the School, the Werner Chemical Society, international chemical societies, allied institutions and/or the Institute of Chemistry of Ireland. You will find many of them interesting and valuable. Attendance at these lectures is recorded.

Please read this document carefully, paying particular attention to Appendices 1-4

Structure of the Senior Sophister Year

During semester 1 students will focus on self-directed learning for the development of their problem-solving skills and on research work towards completion of their capstone project.

Activities in semester 1 will be assessed via viva-voce examination during the Semester-1 assessment week.

In semester 1 students will be given one problem-solving assignment with a total of 6 problems. Students will be expected to solve the problems individually and are encouraged to consult textbooks and scientific literature to work on their solutions. Needless to say, you are not allowed to copy solutions from other students or work on the problems in groups. After submission of your coursework, you are free to discuss the problems with others.

Students are to submit **two** hard copies of their solutions (if handwritten, please include a photocopy) to the School Office **by 16:30 on Tuesday 30 October**. Students carrying out their project abroad will be asked to submit their solutions via email to the main office (farrea25@tcd.ie) by the same date (pdf format, either typed or handwritten scanned copies).

Viva-voce examination for problem-solving component: This section of the viva will be 10 minutes long and will take place after the discussion of the project is closed. The assessors will select one of the six problems in the assignment and will ask the student to solve either the problem or a section of it during the examination (pen and paper or blackboard) and discuss/articulate the approach taken. Students will be encouraged to identify and correct any mistakes made in their original submissions.

You must attend all of those lectures listed as **core** modules together with **four topics** chosen from the list of options (if a Chemistry student) or **three topics** (if a CMM student). A list of all available modules is included in this handbook. Chemistry and CMM students must notify the School Office electronically of the topics you will take by Wednesday **5 December 2018**.

All students are required to attend the School Research Seminars that are held during the year (Thursdays at 12 noon) and should also attend any research lectures organized by the Werner Chemical Society.

Moderatorship Examinations

Your examination timetable will be available through your student portal (my.tcd.ie) at least four weeks before the start of the exam period.

All degree programmes except N-PCAM will use the same set of external examiners. They review the exam questions and the structure of the exam papers before they are finalized. They also review exam scripts and project theses.

The School's external examiners in 2018/19 are as follows:

Organic Chemistry:	Prof. David J. Procter (Manchester)
Inorganic Chemistry:	Prof. Michael Hardie (Leeds)
Physical Chemistry:	Prof. Stuart Mackenzie (Oxford)
Medicinal Chemistry:	Prof. Carmen Galan (Bristol)
CMM:	Prof. Rob Jackson (Keele)
N-PCAM:	Prof. Magdalena Titirici (Queen Mary University of London)

The external examiners will be in the School in May 2019 (dates to be confirmed) and they may request a viva voce with any candidate. It is likely that all Senior Sophisters will be asked to attend on the morning of the interviews, with those being called for a viva being notified at that meeting.

You cannot conclude anything about your performance in the examinations by being called to a viva.

You must ensure that you are available if you are called for interview by the External Examiners.

Moderatorship in Chemistry

The SS year has a total of 60 ECTS, broken down as follows:

Project mark:	20 credits	33.33%
Problem-solving viva	1 credit	1.67%
Examinations:	39 credits	65%

The final degree mark will comprise 35% from your JS mark and 65% from your SS mark. There will be a 1.5-hour moderatorship examination for 5-ECTS modules that are assessed by examination and a 3-hour examination for 10-ECTS modules, with each 5-ECTS paper being worth 8.3% of the overall mark for the SS year (16.67% for 10-ECTS modules/exams). The mark from the problem-solving viva question will contribute 10% to the mark for CHU44108.

Core Lecture Modules

CHU44104 - Advanced Inorganic Chemistry 1 (Chem) (5 ECTS)	Contact Hours
Advanced Inorganic Materials Chemistry	11L
Characterisation Techniques in Bioinorganic Chemistry	11L

CHU44105 - Advanced Inorganic Chemistry 2 (Chem, CMM) (5 ECTS)	Contact Hours
Heavy Transition Metals	11L
Advanced Coordination Chemistry	11L

CHU44167 - Advanced Physical Chemistry (C, CMM, N-PCAM) (10 ECTS)	Contact Hours
Solid State	11L
Photochemistry	11L
Quantum Chemistry	11L
Advanced Physical Chemistry	11L

CHU44108 Chemistry Advanced Topics and Problem-Solving (Chem) (10 ECTS)	Contact Hours
*Advanced Organometallics (CHU44014)	8L
Matter Transport in Solids (CHU44022)	10L
Quantum Chemistry (CHU44023)	8L
Supramolecular Chemistry (CHU44025)	8L
Topics in Structural Chemistry (CHU44027)	8L
Organic Synthetic Methods II (CHU44031)	8L
DNA Structure and Drug—DNA complexes (CHU44034)	8L
Chemical Biology (CHU44036)	8L
Introduction to Static and Dynamic Atomistic Simulation (CHU44063)	10L
Molecular Informatics (CHU44080)	8L
Problem-solving (Self-directed and online learning)	

*New in 2018/19

CHU44113 - Advanced Organic Transformations (Chem, MedChem) (10 ECTS)	Contact Hours
Advanced Organic Transformations I	21L
Advanced Organic Transformations II (Retrosynthesis)	13L
Advanced Organic Transformations II (Asymmetric Synthesis)	10L

Note: The number of contact hours may differ slightly from those indicated above

CHU44108 Topics

You must choose **four** topics (each credited as 1.25 units) from the list given below, and **you must notify the School Office by email to AnneMarie Farrell (farrea25@tcd.ie) of your choice by Wednesday 5 December 2018**. You will be contacted about this during the semester. Please note that option topics that have been requested by only a few students may not go ahead.

CHU44014 Advanced organometallics: New methods and synthetic approaches in modern organometallic chemistry. New ligands in organometallic chemistry. Stabilisation of unusual oxidation states. Organometallic chemistry of water. Bio-organometallic chemistry.

- CHU44022 Matter transport in solids:** Ionic conductance and diffusion processes in solids considered from first principles; applications include solid state reactions, including corrosion of metals and alloys, and fast ion conductors and their uses in advanced battery systems and chemical sensors.
- CHU44023 Quantum chemistry:** Quantum operators; perturbation theory and applications (Stark effect); beyond the Hartree-Fock limit; vibrations in solids (phonons).
- CHU44025 Supramolecular chemistry:** Host–guest chemistry and molecular recognition, including relevance to biological processes and 'molecular engineering'. Self-assembly and anion sensing.
- CHU44027 Topics in structural chemistry:** A brief review of the preparation, structural chemistry and physico-chemical properties of (i) molecular crystals and (ii) copper oxide superconductors, emphasising the interplay between composition, structure and properties.
- CHU44031 Organic synthetic methods:** This course is concerned with the mode of action and the synthesis of the microtubule active anti-cancer agents Taxol[®] and Epothilone.
- CHU44034 DNA structure and drug—DNA complexes:** Spectroscopic tools for studying nucleic acids; structure of DNA (A, B and Z); covalent and non-covalent binding to DNA; relevance to drug design.
- CHU44036 Chemical biology (MOS).** Development of bioorganic chemistry: Classic approach, biosynthetic studies, structure elucidations, enzyme models; overview chemical biology; catalytic antibodies; ribozymes and RNA world; directed evolution; combinatorial libraries; concepts in genomics, proteomics, metabolomics; nanotherapeutics and nanobiomedicine.

CHU44063 Introduction to static and dynamic atomistic simulation (DMacD/JC). An introduction to a simple yet powerful method for solving the many particle equations of motion for molecular systems; applications in chemistry.

CHU44080 Molecular informatics (DMacD)

“If you want to understand life, don't think about throbbing gels and oozes, think about information technology”, Richard Dawkins, in: *The Blind Watchmaker*, 1986.

The interface of the molecular and computational sciences has traditionally been concerned with the application of computers to solve problems, or calculate properties of interest, in physics, chemistry and biology. This topic reverses the paradigm and explores how molecular processes may be employed to perform calculations, and even how some biochemical processes may formally correspond to computational processes.

Some aspects of molecular technology, both synthetic and natural, which relate to computing will be considered, including: (i) Computing with molecules (including Adleman's demonstration of computing with DNA); (ii) Error-coding in molecular recognition (or how concepts employed in error detection in digital TV are also found in biology) and (iii) Molecular Logic Gates – chemical systems that mimic the conventional logic gates underlying electronic circuitry.

CHU44120 Chemistry Capstone Project (20 ECTS)

This module is discussed in detail above.

CHEMISTRY SEMINARS: 12 o'clock on Thursdays in the CHLLT

ALL SS STUDENTS HAVE TO ATTEND THESE

*Other or additional topics may be offered at a later date.

Moderatorship in Medicinal Chemistry

The SS year has a total of 60 ECTS, broken down as follows:

Project mark:	20 credits	33.33%
Problem-solving viva	1 credit	1.67%
Examinations:	39 credits	65%

The final degree mark will comprise 35% from your JS mark and 65% from your SS mark. There will be a 1.5-hour moderatorship examination for 5-ECTS modules that are assessed by examination and a 3-hour examination for 10-ECTS modules, with each 5-ECTS paper being worth 8.3% of the overall mark for the SS year (16.67% for 10-ECTS modules/exams). The mark from the problem-solving viva question will contribute 10% to the mark for CHU44408.

Core Lecture Modules

CHU44113 - Advanced Organic Transformations (Chem, MedChem) (10 ECTS)	Contact Hours
Advanced Organic Transformations I	21L
Advanced Organic Transformations II (Retrosynthesis)	13L
Advanced Organic Transformations II (Asymmetric Synthesis)	10L

CHU44401- Advanced MedChem 1 (MedChem) (10 ECTS)	Contact Hours
Central Nervous System	22L
Computational Medicinal Chemistry	11L
Analytical methods	10L

CHU44402- Advanced MedChem 2 (MedChem) (10 ECTS)	Contact Hours
Site-specific Drug Delivery Systems	11L
Combinatorial Chemistry & Screening Methods	11L
The Cardiovascular System	11L
Case Studies	11L

CHU44408 MedChem Advanced Topics and Problem-Solving (MedChem) (10 ECTS)	Contact Hours
Supramolecular Chemistry (CHU44025)	8L
Organic Synthetic Methods II (CHU44031)	8L
DNA Structure and Drug—DNA complexes (CHU44034)	8L
Chemical Biology (CHU44036)	8L
Problem-solving (Self-directed and online learning)	

Note: The number of contact hours may differ slightly from those indicated above

Topics

CHU44408 Advanced Medicinal Chemistry V (5 ECTS)

These topics have been selected from the option topics for TR071 students as being particularly appropriate to Medicinal Chemists:

CHU44025 Supramolecular chemistry: Host–guest chemistry and molecular recognition, including relevance to biological processes and 'molecular engineering'. Self-assembly and anion sensing.

CHU44031 Organic synthetic methods: This course is concerned with the mode of action and the synthesis of the microtubule active anti-cancer agents Taxol[®] and Epothilone.

CHU44034 DNA structure and drug—DNA complexes: Spectroscopic tools for studying nucleic acids; structure of DNA (A, B and Z); covalent and non-covalent binding to DNA; relevance to drug design.

CHU44036 Chemical biology: Development of bioorganic chemistry: Classic approach, biosynthetic studies, structure elucidations, enzyme models; overview chemical biology; catalytic antibodies; ribozymes and RNA world; directed evolution; combinatorial libraries; concepts in genomics, proteomics, metabolomics; nanotherapeutics and nanobiomedicine.

CHU44420 MedChem Capstone Project (20 ECTS)

This module is discussed in detail above.

**CHEMISTRY SEMINARS 12 o'clock on Thursdays in the CHLLT;
ALL SS STUDENTS HAVE TO ATTEND THESE**

Moderatorship in Chemistry with Molecular Modelling

The SS year has a total of 60 ECTS, broken down as follows:

Project mark:	20 credits	33.33%
Problem-solving viva	1 credit	1.67%
Examinations:	39 credits	65%

The final degree mark will comprise 35% from your JS mark and 65% from your SS mark. There will be a 1.5-hour moderatorship examination for 5-ECTS modules that are assessed by examination and a 3-hour examination for 10-ECTS modules, with each 5-ECTS paper being worth 8.3% of the overall mark for the SS year (16.67% for 10-ECTS modules/exams). The mark from the problem-solving viva question will contribute 10% to the mark for CHU44708.

Core Lecture Modules

CHU44105 - Advanced Inorganic Chemistry 2 (Chem, CMM) (5 ECTS)	Contact Hours
Heavy Transition Metals	11L
Advanced Coordination Chemistry	11L

CHU44167 - Advanced Physical Chemistry (C, CMM, N-PCAM) (10 ECTS)	Contact Hours
Solid State	11L
Photochemistry	11L
Quantum Chemistry	11L
Advanced Physical Chemistry	11L

CHU44112 - Advanced Organic Transformations I (CMM) (5 ECTS)	Contact Hours
Advanced Organic Transformations I	21L

CHU44701 Advanced CMM (CMM) (10 ECTS)	Contact Hours
Computational Medicinal Chemistry	11L
High Performance Computing	11L
Computational Molecular Quantum Chemistry	11L
Advanced Molecular Dynamics	11L

CHU44708 CMM Advanced Topics and Problem-Solving (CMM)(10 ECTS)	Contact Hours
*Advanced Organometallics (CHU44014)	8L
Matter Transport in Solids (CHU44022)	10L
**Quantum Chemistry (CHU44023)	8L
Supramolecular Chemistry (CHU44025)	8L
Topics in Structural Chemistry (CHU44027)	8L
Organic Synthetic Methods II (CHU44031)	8L
DNA Structure and Drug—DNA complexes (CHU44034)	8L
Chemical Biology (CHU44036)	8L
Molecular Informatics (CHU44080)	8L
Problem-solving (Self-directed and online learning)	

*New in 2018/19

**Mandatory topic

Note: The number of contact hours may differ slightly from those indicated above

CHU44708 Option Module & Problems Solving

You must take one topic (CHU44023, Quantum chemistry) and choose any **three** other topics (each credited as 1.25 units) from the list given below*. **You must notify the School office by email to AnneMarie Farrell (farrea25@tcd.ie) of your choice by Wednesday 5 December 2018.**

More information will be made available during the semester. Please note that option topics that have been requested by only a few students may not be offered. Students interested in Medicinal Chemistry will find courses CHU44031-CHU44036 especially appropriate.

CHU44014 Advanced organometallics: New methods and synthetic approaches in modern organometallic chemistry. New ligands in organometallic chemistry. Stabilisation of

unusual oxidation states. Organometallic chemistry of water. Bio-organometallic chemistry.

CHU44022 Matter transport in solids: Ionic conductance and diffusion processes in solids considered from first principles; applications include solid state reactions, including corrosion of metals and alloys, and fast ion conductors and their uses in advanced battery systems and chemical sensors.

CHU44023 Quantum chemistry: Quantum operators; perturbation theory and applications (Stark effect); beyond the Hartree-Fock limit; vibrations in solids (phonons).

CHU44025 Supramolecular chemistry: Host–guest chemistry and molecular recognition, including relevance to biological processes and 'molecular engineering'. Self-assembly and anion sensing.

CHU44027 Topics in structural chemistry: A brief review of the preparation, structural chemistry and physico-chemical properties of (i) molecular crystals and (ii) copper oxide superconductors, emphasising the interplay between composition, structure and properties.

CHU44031 Organic synthetic methods: This course is concerned with the mode of action and the synthesis of the microtubule active anti-cancer agents Taxol[®] and Etoposide.

CHU44034 DNA structure and drug—DNA complexes: Spectroscopic tools for studying nucleic acids; structure of DNA (A, B and Z); covalent and non-covalent binding to DNA; relevance to drug design.

CHU44036 Chemical biology: Development of bioorganic chemistry: Classic approach, biosynthetic studies, structure elucidations, enzyme models; overview chemical biology; catalytic antibodies; ribozymes and RNA world; directed evolution; combinatorial libraries; concepts in genomics, proteomics, metabolomics; nanotherapeutics and nanobiomedicine.

CHU44037 Electrochemical biosensors: The physical principles underlying electrochemical sensors. A survey of surface-immobilized redox-enzyme-based biosensor devices using electrochemical transduction. Strategies for enzyme wiring. Self-assembled monolayer-based biosensors.

CHU44080 Molecular informatics:

“If you want to understand life, don't think about throbbing gels and oozes, think about information technology”, Richard Dawkins, in: *The Blind Watchmaker*, 1986. The interface of the molecular and computational sciences has traditionally been concerned with the application of computers to solve problems, or calculate properties of interest, in physics, chemistry and biology. This topic reverses the paradigm and explores how molecular processes may be employed to perform calculations, and even how some biochemical processes may formally correspond to computational processes.

Some aspects of molecular technology, both synthetic and natural, which relate to computing will be considered, including: (i) Computing with molecules (including Adleman's demonstration of computing with DNA); (ii) Error-coding in molecular recognition (or how concepts employed in error detection in digital TV are also found in biology) and (iii) Molecular Logic Gates – chemical systems that mimic the conventional logic gates underlying electronic circuitry.

CHU44720 CMM Capstone Project (20 ECTS)

This module is discussed in detail above.

CHEMISTRY SEMINARS 12 o'clock on Thursdays in the CHLLT
ALL SS STUDENTS HAVE TO ATTEND THESE

Other or additional option topics may be offered at a later date.

Components contributing to module marks

All 5-ECTS modules will have a 1.5-hour examination as part/all of their assessment, while 10-ECTS modules will have a 3-hour examination.

The contributions of components to overall module marks are as follows:

Module Code	ECTS	Mark Component Number	Mark Component Description	Contribution to overall mark (%)
CHU44104	5	1	Exam component	100
CHU44105	5	1	Exam component	100
CHU44167	10	1	Exam component	100
CHU44108/ CHU44408/ CHU44708	10	1	Exam component	90
		2	Viva Component	10
CHU44112	5	1	Exam component	100
CHU44113	10	1	Exam component	100
CHU44401	10	1	Exam component	100
CHU44402	10	1	Exam component	100
CHU44601	5	1	Exam component	100
CHU44701	10	1	Exam component	100
CHU44120/ CHU44420/ CHU44720	20	1	Project Report and Viva	
			Supervisor's mark (project & report only)	20
			Internal Assessor 1's mark	40
			Internal Assessor 2's mark	40

Prizes

Cocker Prize in Chemistry

This prize was founded in 1949 by a gift from Sir William W. Cocker, O.B.E., LL.D. (h.c.). Provided sufficient merit is shown, the prize is awarded annually by the Board on the recommendation of the Head of the School of Chemistry to the student taking a moderatorship in chemistry, medicinal chemistry or chemistry with molecular modelling who shows the greatest practical ability during his or her Senior Sophister year. If income permits additional prizes, or a prize of greater value, may be awarded. Value, €760 and a silver medal.

Henderson-Lloyd Prize in Advanced Materials

This prize is awarded to the student who has obtained the highest marks in the moderatorship examination in nanoscience, physics and chemistry of advanced materials. Dr B. Henderson was formerly Erasmus Smith's Professor of Natural and Experimental Philosophy, Dr D.R. Lloyd was University Professor of Chemistry, and together they were instrumental in establishing the materials moderatorship in Trinity College Dublin. The prize is awarded on the recommendation of the Director of Nanoscience, Physics and Chemistry of Advanced Materials. Value, €508.

W.H.A. Macintosh Prize

This prize was founded by a legacy from Mr W.H.A. Macintosh, former chief technician in the Department of Chemistry. It is awarded annually to the student who is proceeding directly from moderatorship to undertake research in the School of Chemistry, leading to a Ph.D. in inorganic, organic or physical chemistry, and who has obtained the highest mark in his or her chemistry moderatorship examination. Value, €635.

Gold Medal

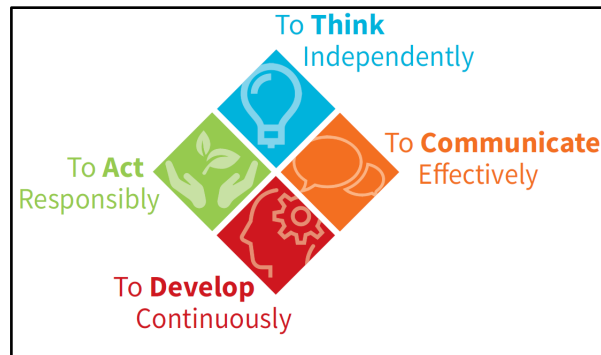
Gold medals are awarded by the Board to candidates of the first class who have shown exceptional merit at the degree examination in honor or professional courses (see www.tcd.ie/academicregistry/exams).

Graduate Attributes

The Trinity Graduate Attributes represent the qualities, skills and behaviours that you will have the opportunity to develop as a Trinity student over your entire university experience, in other words, not only in the classroom, but also through engagement in co- and extra-curricular activities (such as summer work placements, internships, or volunteering).

The four Trinity Graduate Attributes are:

- To Think Independently
- To Act Responsibly
- To Develop Continuously
- To Communicate Effectively



Why are the Graduate Attributes important?

The Trinity Graduate Attributes will enhance your personal, professional and intellectual development. They will also help to prepare you for lifelong learning and for the challenges of living and working in an increasingly complex and changing world.

The Graduate Attributes will enhance your employability. Whilst your degree remains fundamental, also being able to demonstrate these Graduate Attributes will help you to differentiate yourself as they encapsulate the kinds of transversal skills and abilities, which employers are looking for.

How will I develop these Graduate Attributes?

Many of the Graduate Attributes are 'slow learned', in other words, you will develop them over the four or five years of your programme of study.

They are embedded in the curriculum and in assessments, for example, through undertaking independent research for your final year project, giving presentations and engaging in group work.

You will also develop them through the co-curricular and extra-curricular activities. If you help to run a club or society you will be improving your leadership skills, or if you play a sport you are building your communication and team-work skills.

Useful links to College services and support

- A full listing of support services can be found at <http://www.tcd.ie/students/supports-services/>
- The Senior Tutor's website is <https://www.tcd.ie/seniortutor/>
- The Students Union can be found at <https://www.tcdsu.org/>, with student representation structures detailed at <https://www.tcdsu.org/aboutus>
- A full listing of societies can be found at <http://trinitysocieties.ie/> and sports information is at http://www.tcd.ie/Sport/student-sport/ducac/?nodeId=94&title=Sports_Clubs
- The Academic Registry is at <https://www.tcd.ie/academicregistry/>
- Information and community for mature students can be accessed at <https://www.tcd.ie/maturestudents/>
- Details of how your data will be handled under GDPR (General Data Protection Rules) are available at https://www.tcd.ie/info_compliance/data-protection/student-data/

Relevant University Regulations

[Academic Policies](#)

[Student Complaints Procedure](#)

[Dignity & Respect Policy](#)

[Student Partnership Policy](#)

Appendix 1: Examination Regulations

1. General College Regulations

General College regulations with regard to examinations shall apply to all examinations in Science as set out in the University Calendar 2018-19 (available for download from each JS webpage – see URLs on p.1)

2. Examination Regulations

- 2.1. Examination timetables will be published on the portal <https://my.tcd.ie> four weeks prior to examinations taking place.

The College reserves the right to alter the published time and date of an examination in exceptional circumstances. Students should ensure that they are available for examinations for the duration of the relevant examination session as stated in the Almanack.

This following extract is taken from the general [regulations and information section](#) of the 2018/19 College Calendar:

67 Students must obtain credit for the academic year by satisfactory attendance at lectures and tutorials and by carrying out, submitting and sitting the required assessment components. In addition, students must pass the year by achieving, at a minimum, an overall credit-weighted average pass mark for the year (40 per cent or 50 per cent, as per programme regulations) and either:

(a) accumulate 60 credits by achieving at least the pass mark in all modules

or

(b) **Pass by Compensation.** All modules and components within modules are compensatable (except in particular professional programmes where compensation does not apply). To pass a year by compensation, in programmes that locate the pass mark at 40 per cent, a student must

achieve the pass mark in modules carrying a minimum of 50 credits and obtain a module mark of at least 35 per cent in any remaining module(s). A student may accumulate a maximum of 10 credits at qualified pass where the mark lies between 35-39 per cent.

The end of year or degree result moderated by the court of examiners must be returned and recorded on the student record.

68 Progression is on an annual basis. Within a year students may carry failed modules from one semester to the next but not from one academic year to another; that is, they will not be able to rise to the next year of their programme until they have successfully completed the preceding year(s). Students who have not passed their year are required to present for reassessment when:

- (a) they obtain in excess of 10 credits at qualified pass (i.e. marks between 35-39 per cent where the pass mark is 40 per cent;
- (b) they fail any module (i.e. achieving marks below 35 per cent where the pass mark is 40 per cent; or below 45 per cent where the pass mark is 50 per cent);
- (c) they do not obtain an overall pass mark for the year;
- (d) any combination of (a) - (c) occurs.

69 If a student has achieved both fail and qualified pass grades at the first sitting or has exceeded the 10 credit limit allowed for compensation and is not permitted to rise with their year, they must present for reassessment in all failed components of all modules for which they obtained a fail and/or a qualified pass.

70 Different modalities of assessment to the first sitting are permitted in the reassessment session as determined by the programme.

71 The same compensation regulations as outlined above apply at the reassessment session.

72 Students who fail to satisfy the requirements of their year at the reassessment session are required to repeat the year in full (i.e. all modules and all assessment components).

73 Students are permitted to repeat any year of an undergraduate programme subject to not repeating the same year more than once and not repeating more than two academic years within a degree course, except by special permission of the University Council.

74 The maximum number of years to complete an undergraduate degree is six years for a standard four-year programme and seven years for a five-year programme.

75 Under certain conditions approved by the University Council, on the recommendation of the Senior Lecturer in consultation with the appropriate head(s) of school(s), director(s) of undergraduate teaching and learning, head(s) of department(s), Associate Dean for Undergraduate Science Education or course director, the University regards attendance at courses and the passing of approved examinations in other colleges as fulfilling or partially fulfilling the exercises required for certain degrees of the University. Where places are available students may be permitted advanced entry to their course, if they are deemed qualified by their knowledge and attainment to do so, or by passing specified examinations. Applicants must pay a fee before presenting themselves for examination (see COLLEGE CHARGES). Applications for advanced entry to any course should be made through the [Academic Registry](#) in the first instance.

76 Students must pursue their undergraduate course continuously unless they are permitted by the Senior Lecturer to interrupt it, normally for a period of one year, either by going 'off-books' or by intermitting their studies for extra-curricular reasons.

Absence from Examinations ([taken from Calendar general regulations and information](#))

44 Students who may be prevented from sitting an examination or examinations (or any part thereof) due to illness should seek, through their tutor, permission from the Senior Lecturer in advance of the examination session to defer the examination/s to the reassessment session. Students who have commenced the examination session, and are prevented from completing the session due to illness should seek, through their tutor, permission from the Senior Lecturer to defer the outstanding examination/s to the reassessment session.

45 Where such permission is sought, it must be appropriately evidenced:

(a) For illness: medical certificates must state that the student is unfit to sit examinations/ complete assessment and specify the date(s) of the illness and the dates on which the student is

not fit to sit examinations/complete assessment. Medical certificates must be submitted to the student's tutor within three days of the beginning of the period of absence from the assessment/examination.

(b) For other grave cause: appropriate evidence must be submitted to the student's tutor within three days of the beginning of the period of absence from the assessment/examination.

46 Where illness occurs during the writing of an examination paper, it should be reported immediately to the chief invigilator. The student will then be escorted to the College Health Centre. Every effort will be made to assist the student to complete the writing of the examination paper.

47 Where an examination/assessment has been completed, retrospective withdrawal will not be granted by the Senior Lecturer nor will medical certificates be accepted in explanation for poor performance.

Appendix 2: Description of the European Credit Transfer System (ECTS)

The European Credit Transfer and Accumulation System (ECTS) is an academic credit system based on the estimated student workload required to achieve the objectives of a module or programme of study. It is designed to enable academic recognition for periods of study, to facilitate student mobility and credit accumulation and transfer. The ECTS is the recommended credit system for higher education in Ireland and across the European Higher Education Area.

The ECTS weighting for a module is a **measure of the student input or workload** required for that module, based on factors such as the number of contact hours, the number and length of written or verbally presented assessment exercises, class preparation and private study time, laboratory classes, examinations, clinical attendance, professional training placements, and so on as appropriate. There is no intrinsic relationship between the credit volume of a module and its level of difficulty.

The European **norm for full-time study over one academic year is 60 credits**. A credit value of 1 ECTS represents 20-25 hours of estimated student input, so a 10-credit module will be designed to require 200-250 hours of student input including class contact time and assessments.

ECTS credits are awarded to a student only upon successful completion of the course year. Progression from one year to the next is determined by the course regulations. Students who fail a year of their course will not obtain credit for that year even if they have passed certain component courses. Exceptions to this rule are one-semester and one-year visiting students, who are awarded credit for individual modules successfully completed.

Appendix 3: College regulation regarding plagiarism

Simply put, plagiarism is the presentation of the work of someone as your own - the university takes plagiarism offences extremely seriously. Information on what constitutes plagiarism and how the university deals with it can be found in the central repository on plagiarism (<http://tcd-ie.libguides.com/plagiarism>) and in the Plagiarism Policy document_QPOLPlag, which will be made available on your course website.

All students must complete our [Ready Steady Write plagiarism tutorial](#) and sign a declaration when submitting course work, whether in hard or soft copy or via Blackboard, confirming that you understand what plagiarism is and have completed the tutorial.

Extract from the College Calendar 2018/19

96 General

It is clearly understood that all members of the academic community use and build on the work and ideas of others. It is commonly accepted also, however, that we build on the work and ideas of others in an open and explicit manner, and with due acknowledgement.

Plagiarism is the act of presenting the work or ideas of others as one's own, without due acknowledgement.

Plagiarism can arise from deliberate actions and also through careless thinking and/or methodology. The offence lies not in the attitude or intention of the perpetrator, but in the action and in its consequences.

It is the responsibility of the author of any work to ensure that he/she does not commit plagiarism.

Plagiarism is considered to be academically fraudulent, and an offence against academic integrity that is subject to the disciplinary procedures of the University.

97 Examples of Plagiarism

Plagiarism can arise from actions such as:

- (a) copying another student's work;
- (b) enlisting another person or persons to complete an assignment on the student's behalf;
- (c) procuring, whether with payment or otherwise, the work or ideas of another;
- (d) quoting directly, without acknowledgement, from books, articles or other sources, either in printed, recorded or electronic format, including websites and social media;
- (e) paraphrasing, without acknowledgement, the writings of other authors.

Examples (d) and (e) in particular can arise through careless thinking and/or methodology where students:

- (i) fail to distinguish between their own ideas and those of others;
- (ii) fail to take proper notes during preliminary research and therefore lose track of the sources from which the notes were drawn;
- (iii) fail to distinguish between information which needs no acknowledgement because it is firmly in the public domain, and information which might be widely known, but which nevertheless requires some sort of acknowledgement;
- (iv) come across a distinctive methodology or idea and fail to record its source. All the above serve only as examples and are not exhaustive.

98 Plagiarism in the context of group work

Students should normally submit work done in co-operation with other students only when it is done with the full knowledge and permission of the lecturer concerned. Without this, submitting work which is the product of collaboration with other students may be considered to be plagiarism.

When work is submitted as the result of a group project, it is the responsibility of all students in the group to ensure, so far as is possible, that no work submitted by the group is plagiarised. In order to avoid plagiarism in the context of collaboration and group work, it is particularly important to ensure that each student appropriately attributes work that is not their own.

99 Self plagiarism

No work can normally be submitted for more than one assessment for credit. Resubmitting the same work for more than one assessment for credit is normally considered self-plagiarism.

100 Avoiding plagiarism

Students should ensure the integrity of their work by seeking advice from their lecturers, tutor or supervisor on avoiding plagiarism. All schools and departments must include, in their handbooks or other literature given to students, guidelines on the appropriate methodology for the kind of work that students will be expected to undertake. In addition, a general set of guidelines for students on avoiding plagiarism is available on <http://tcd-ie.libguides.com/plagiarism>.

Appendix 4: Mark scheme and schedule of grades in Sophister years

Mark Range	Criteria
90-100	IDEAL ANSWER ; showing insight and originality and wide knowledge. Logical, accurate and concise presentation. Evidence of reading and thought beyond course content. Contains particularly apt examples. Links materials from lectures, practicals and seminars where appropriate.
80-89	OUTSTANDING ANSWER ; falls short of the 'ideal' answer either on aspects of presentation or on evidence of reading and thought beyond the course. Examples, layout and details are all sound.
70-79	MAINLY OUTSTANDING ANSWER ; falls short on presentation and reading or thought beyond the course, but retains insight and originality typical of first class work.
65-69	VERY COMPREHENSIVE ANSWER ; good understanding of concepts supported by broad knowledge of subject. Notable for synthesis of information rather than originality. Sometimes with evidence of outside reading. Mostly accurate and logical with appropriate examples. Occasionally a lapse in detail.
60-64	LESS COMPREHENSIVE ANSWER ; mostly confined to good recall of coursework. Some synthesis of information or ideas. Accurate and logical within a limited scope. Some lapses in detail tolerated.
55-59	SOUND BUT INCOMPLETE ANSWER ; based on coursework alone but suffers from a significant omission, error or misunderstanding. Usually lacks synthesis of information or ideas. Mainly logical and accurate within its limited scope and with lapses in detail.
50-54	INCOMPLETE ANSWER ; suffers from significant omissions, errors and misunderstandings, but still with understanding of main concepts and showing sound knowledge. Several lapses in detail.
45-49	WEAK ANSWER ; limited understanding and knowledge of subject. Serious omissions, errors and misunderstandings, so that answer is no more than adequate.
40-44	VERY WEAK ANSWER ; a poor answer, lacking substance but giving some relevant information. Information given may not be in context or well explained, but will contain passages and words, which indicate a marginally adequate understanding.
35-39	MARGINAL FAIL ; inadequate answer, with no substance or understanding, but with a vague knowledge relevant to the question.
30-34	CLEAR FAIL ; some attempt made to write something relevant to the question. Errors serious but not absurd. Could also be a sound answer to the misinterpretation of a question.
0-29	UTTER FAIL ; with little hint of knowledge. Errors serious and absurd. Could also be a trivial response to the misinterpretation of a question.

Schedule of Grades

I	=70%+
II-1	= 60-69%
II-2	= 50-59%
III	= 40-49%
F-1	= 30-39%
F-2	= 0-29%
U.G.	= Ungraded

In the event of any conflict or inconsistency between the General Regulations published in the University Calendar and information contained in this handbook, the provisions of the General Regulations in the Calendar will prevail (Calendar, Part II, [General Regulations and Information](#), Section II, Item 12).

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Date of next review: Academic Year 2019/20