Descriptors for Modules Taught as part of Dublin Chemistry's Structured Ph.D. Programme

Contents

* Compulsory Module

CHEM40210 – Comprehensive X-ray Crystallography

Short Title	Long Title
Comp X-ray Crystallography	Comprehensive X-ray Crystallography

Level	Credits	Semester	Passing Grade	Module Coordinator
4	2.5	Semester Two	DPF	Helge Müller-Bunz (UCD- Sylvia Draper, Wolfgang Schmitt (TCD)

Total Places	Core /Option
20	20

Module Description
The module aims to give students the opportunity to develop a theoretical, analytical and practical approach to the use of X-ray Crystallography. Students will be aware of the format for reporting data and learn to appreciate the quality of published data.

Learning Outcomes
On successful completion of this module, students should:· Have a knowledge and understanding of the theoretical principles underpinning X-ray Crystallography;· Be familiar with operational constraints of the technique; Be familiar with the use of a polarizing microscope to determine crystals suitable for analysis;· Be able to read and understand data tables;· Be able to analyse and interpret data and be able to discern how reliable finished data tables are;· Be able to present data in a form suitable for publication in a thesis or manuscript;· Be aware of quality of published data in literature. Course is Graded as Pass (60%) or Distinction (76%).

Workload

Type	Hours
Lectures	10
Autonomous Student Learning	25
Tutorial	3
Laboratories	2
Specified Learning Activities	10
Total	**50**

Assessment Details

Description	Timing	Score By	% Final Grade	In Blackboard ?
< Description >	End_Sem_Sub	LET	100	N
Total			**100**	

CHEM40240 – Spectroscopic Techniques

Short Title	Long Title
Spectro Techniques (TCD)	Spectroscopic Techniques (TCD)

Level	Credits	Semester	Passing Grade	Module Coordinator
4	2.5	Semester One	DPF	Susan Quinn, UCD Sylvia Draper, Yurii Gun'ko, TCD

Total Places	Core /Option
35	35

Module Description

The module aims to give students the opportunity to develop a theoretical, analytical and practical approach to the use of spectroscopic techniques. It includes content related to: the physical principles underlying the techniques, instrument operational parameters and application to various chemical and biological systems. The techniques covered include Infrared (IR), near infrared (NIR), Raman, UV-visible, Circular Dichroism and Emission spectroscopy. These techniques will be taught from the perspective of theory, spectral output and compound analysis. The scope of the course will include sample type, preparation, spectrometer parameters and nature of the spectral experiment, and analyses of the spectral output. Students are exposed to each technique in a systematic and in-depth way. The emphasis is on the application of spectroscopy in the laboratory.

Learning Outcomes

On successful completion of this module, students should:·
Have a knowledge and understanding of the theoretical principles underpinning general spectroscopic techniques used routinely in Industry;·
Be familiar with the operational constraints of each technique;·
Be aware of sampling procedures;·
Be able to analyse and interpret data and have an appreciation of the limitations of the each spectroscopic technique·;
Be capable of designing a method combining different techniques·
Be able to identify the most suitable spectroscopic techniques for the analysis of a given sample

Course is Graded as Pass (60%) or Distinction (76%)

Workload

Type	Hours
Autonomous Student Learning	16
Lectures	10
Specified Learning Activities	20
Seminar	4
Total	**50**

Assessment Details

Description	Timing	Score By	% Final Grade	In Blackboard ?
Literature survey	Varies	MRK	50	N
Technique based presentation	Varies	MRK	50	N
Total			**100**	

CHEM40250 – Structure & Biophysical Studies of Nucleic Acids

Short Title	Long Title
Struc&BioStud Nucl Acids (TCD)	Structure and Biophysical Studies of Nucleic Acids: Drug Binding and More (TCD)

Level	Credits	Semester	Passing Grade	Module Coordinator
4	2.5	Semesters One and Two	DPF	Susan Quinn (UCD), Christine Cardin (University of Reading) Isabel Rozas, John Kelly (TCD)

Total Places	Core /Option
35	35

Module Description

The module aims to give students a comprehensive understanding of nucleic acid structures. The introduction will explore the history of the DNA structure and development of synthetic methods for basic and advanced systems. Attention will focus on the use of techniques such as X-ray crystallography and NMR in resolving nucleic acid structures. Based on the understanding of the structural properties the principles governing small molecule binding interactions such as intercalation, groove-binding and anti-sense therapies will be studied. The characterization of nucleic-acid binding interactions will be thoroughly examined by considering a broad range of techniques, including optical, hydrodynamic and calorimetric techniques. Finally, the processes involved in DNA damage will be studied. This will focus on oxidative and photochemical damage and their biological relevance.

Learning Outcomes

On successful completion of this module, students should:·

Have knowledge of the synthetic procedures used for the preparation of nucleic acids and their analogues

Know the different nucleic acid structures and the molecular interactions governing them

Be familiar with structural transitions in nucleic acids.

Know the physical techniques for characterization of nucleic acids in solution

Understand the principles governing binding interactions to nucleic acid structures and the characterization of these interactions

Be aware of processes involved in DNA damage (oxidative and photochemical)

Course is Graded as Pass (60%) or Distinction (76%)

Workload

Type	Hours
Lectures	10
Specified Learning Activities	20
Autonomous Student Learning	20
Total	**50**

Assessment Details

Description	Timing	Score By	% Final Grade	In Blackboard ?
Literature Project	Varies	MRK	50	N
Written Open Book Examination	End_Sem_Exam_2	MRK	50	N
Total			**100**	

CHEM40270 – Synthesis & Chemical Modification of Nanomaterials

Short Title	Long Title
Synth & Chem Modifof Nano(TCD)	Synthesis and Chemical Modification of Nanomaterials (TCD)

Level	Credits	Semester	Passing Grade	Module Coordinator
4	2.5	Semester Two	DPF	Susan Quinn (UCD) Yurii Gun'ko (TCD)

Total Places	Core /Option
35	35

Module Description
The module aims to give students an overview of the principles underlying the manipulation and modification of solution-based nanomaterials. Emphasis will be placed on the preparation and purification of metallic, semiconducting, magnetic and dendrimer-based nanoparticles and of carbon nanotube systems. The chemical and physical properties of nanomaterials will be considered as a function of modification and preparation parameters.

Learning Outcomes
On successful completion of this module, students should: * Understand the basic principals of the bottom-up approach * Have knowledge and understanding of the main approaches in the synthesis of solution-based nanomaterials * Be familiar with techniques used to modify and purify nanomaterials * Have knowledge of the techniques used to characterise nanomaterials * Have a knowledge of material-dependent properties that are tuneable through synthetic design and modification

Workload

Type	Hours
Lectures	11
Autonomous Student Learning	18
Specified Learning Activities	21
Total	**50**

Assessment Details

Description	Timing	Score By	% Final Grade	In Blackboard ?
Examination	End_Sem_Exam_2	LET	100	N
Total			**100**	

CHEM40310 – Catalytic Asymmetric Synthesis

Short Title	Long Title
Catalytic Asymmetric Synthesis	Catalytic Asymmetric Synthesis

Level	Credits	Semester	Passing Grade	Module Coordinator
4	5.0	Semester Two	DPF	Patrick Guiry, Declan Gilheany (UCD) Stephen Connon (TCD)

Total Places	Core /Option
35	35

Module Description

The module aims to give students an advanced course on an area of synthetic organic chemistry of current importance, namely asymmetric synthesis. The key learning objectives of this module are: (a) To understand the need for asymmetric synthesis and a comparison of the currently used approaches, (b) To be able to apply selected chiral reagents, chiral auxiliaries and chiral catalysts in the asymmetric synthesis of organic compounds, (c) To understand the three-dimensional transition states in each of the above approaches and thus understand why a particular stereoisomer is formed, (d) To be able to apply this methodology as key steps in the total synthesis of molecules of biological interest. The type of asymmetric transformations that will be discussed include C-H, C-C and C-O bond formations. The application of transition metal complexes and organocatalysis to these transformations will be a particular emphasis.

Learning Outcomes

On successful completion of this module, students should:
- Have a knowledge and understanding of modern approaches to asymmetric synthesis;
- Be familiar with applications of transition metal complexes and the importance of recent advances in chiral ligands;
- Be familiar with recent advances in the development and use of organocatalysts for asymmetric synthesis;
- Be able to apply these chirotechnologies as key steps in the preparation of biologically important molecules.

Course is graded as Pass (60%) or Distinction (76%)"

Workload

Type	Hours
Specified Learning Activities	18
Lectures	18
Autonomous Student Learning	54
Total	**90**

Assessment Details

Description	Timing	Score By	% Final Grade
Based on Course Materials and Literature Review x3	Varies	MRK	100
Total			**100**

Module Remediation Strategies

Remediation

If you fail this module you may repeat or substitute where permissible. It is not possible to remediate this Module if the reason for failure is the non-submission or late submission of assignments.

CHEM40340 – Teaching in Higher Education as a Graduate Assistant: Chemistry and Chemical Biology*

Short Title	Long Title
Grad Assistant	Teaching in Higher Education as a Graduate Assistant: Chemistry and Chemical Biology

Level	Credits	Semester	Passing Grade	Module Coordinator
4	5.0		DPF	Andrew Rous, UCD Dónall Mac Dónaill, TCD

Total Places	Core /Option
30	30

Module Description

The module will consist of 3 strands, a practical, a theoretical and a professional. The module will be delivered with a mixture of face-to-face and online environment and participants must be in an active teaching role.

The practical component will consist of an initial presentation on the realities of demonstrating and attendance at a presentation to undergraduates on laboratory safety. There will also be preparatory sessions specific to individual experiments. Although these will be for all demonstrators they will constitute contact hours for those taking this module.

In the theoretical strand, the participants, who are in the role of graduate teaching assistant/demonstrator, will engage in a scholarly critique of their teaching performance in supporting student learning in their disciplinary context. Participants will apply some of the basic generic and discipline-specific skills in their teaching. They will be expected to engage in a scholarly discussion with their peers on best practices in teaching and learning in their context. They will be encouraged to self-assess based on feedback from their peers and/or their students, i.e. encouraged to take responsibility for judging the quality of their teaching.

The professional strand will require that students display a suitable standard of preparation, punctuality, presentation and safety awareness. Administrative competence will also be expected with regard to timely marks entry and custody of laboratory notebooks, which are effectively examination documents.

Learning Outcomes

* Demonstrate knowledge and critique of the principles, relevant policies and techniques of teaching and learning in relation to your own practice and subject area
* Critically evaluate your own teaching and learning approaches and their impact on learners and how they learn
* Take responsibility for planning teaching and learning activities to encourage student engagement in learning and the achievement of specified learning outcomes for each session
* Take responsibility for evaluating your own performance based on feedback from a variety of sources (student, peer, laboratory supervisor) and demonstrate willingness to change approach to demonstrating in light of this feedback
* Demonstrate basic administrative competence.
* Understand the relationship between the design of a practical session and the learning outcomes associated with it.

Course is Graded as Pass, Distinction or Fail

Workload

Type	Hours
Specified Learning Activities	50
Small Group	20
Autonomous Student Learning	20
Lectures	5
Practical	15
Total	**110**

Assessment Details

Description	Timing	Score By	% Final Grade
Curriculum development, using the methodologies discussed in the course to improve teaching		LET	33
Planning (thinking about) my teaching sessions		LET	34
Improving my performance a self relection and analysis of teaching style		LET	33
Total			**100**

Prior Learning

Type	Prior Learning
Recommended	Those participants who started their postgraduate studies in September will be expected to have attended demonstrator training and briefing sessions during the 1st semester.

Required	Participants must: (a) Be, or about to be, registered for PhD/Masters (b) Have, or about to have, an active teaching role

CHEM40350 – Commercialisation of Chemical Research

Short Title	Long Title
Chem Lab to Commercialisation	Chem Lab to Commercialisation

Level	Credits	Semester	Passing Grade	Module Coordinator
4	2.5	Semester One and Two	DPF	Declan Gilheany, UCD Brian Kelly, Celtic Catalysts

Total Places	Core /Option
30	30

Module Description

This module aims to give students an overview of the process of taking an idea/invention in the life sciences from early stage research at the laboratory bench all the way through to a successful and lucrative Company Exit. Topics covered will include industry overview, strategic and business planning, fundraising and real-life case studies.

Learning Outcomes

On successful completion of this module, students should:
-Know the factors required to inform the decision as to how to best commercialise new ideas/inventions developed in the laboratory
-Have an understanding of the various elements required in a Business Plan
-Have an understanding of the various mechanisms involved in funding a business in the life-sciences area
-Have a clear idea of the factors that impact upon value generation and the creation of an investible proposition
-Have a clear understanding of the entrepreneurial environment in Ireland and what supports are/aren't available

Course is Graded as Pass (60%) or Distinction (76%).

Workload

Type	Hours
Lectures	10
Autonomous Student Learning	15
Specified Learning Activities	25
Total	**50**

Assessment Details

Description	Timing	Score By	% Final Grade	In Blackboard ?
Oral/Written	Varies	MRK	50	N
Specific Topic	Varies	MRK	50	N
Total			**100**	

CHEM40360 – Synthesis of Pharmaceutical Compounds

Short Title	Long Title
Advanced Organic Synthesis	Advanced Organic Synthesis

Level	Credits	Semester	Passing Grade	Module Coordinator
4	5.0	Semester Three	DPF	Paul Evans and Mike Casey (UCD)

Total Places	Core /Option
30	30

Module Description

The student following this course will develop an understanding and appreciation of the construction of complex molecules using a variety of chemical methods. They will also be exposed to the different structural types and classes of natural products and, in addition, the link will be made between natural products and pharmaceuticals based on their scaffolds. The course will look in turn at different examples and investigate step-by-step how these compounds may be effectively constructed. During this process the central concepts investigators routinely apply to solve these problems will be illustrated. An emphasis will be placed on problem-based learning and the student will be asked to solve and propose solutions for syntheses and synthetic problems during the class. Students will also approach this overall process themselves in an assignment in which they will propose and design the synthesis of a target molecule that they will finally present to the class. The module is directed towards postgraduate students either following synthetic organic chemistry based research programmes, or with a firm interest in this area.

Learning Outcomes

On completion of this module students should be able to:
- approach rationally the preparation of a complex molecule, possessing multiple functional groups, using the concept of retrosynthetic analysis;
- transfer this rough idea into a feasible forward synthesis taking into account appropriate protecting groups, including an understanding for their selective introduction and removal (orthogonality);
- suggest ways in which to achieve selectivity in the sequence - chemo-, regio- and stereoselectivity.

Course graded as Pass (60%) or Distinction (76%)

Workload

Type	Hours
Specified Learning Activities	24
Lectures	18
Autonomous Student Learning	54
Tutorial	6
Total	**102**

Assessment Details

Description	Timing	Score By	% Final Grade
Literature Asignment	Varies	MRK	50
Retrosynthetic Problem	End_Sem_Sub	MRK	50
Total			**100**

Module Remediation Strategies

Remediation
If you fail this module you may repeat or substitute where permissible. It is not possible to remediate this Module if the reason for failure is the non-submission or late submission of assignments.

CHEM40370 – Advanced NMR Spectroscopy

Short Title	Long Title
Advanced NMR & MS	Advanced NMR & Mass Spectrometry

Level	Credits	Semester	Passing Grade	Module Coordinator
4	5.0	Semester Two	DPF	Yannick Ortin, Patrick Guiry, Andrew Phillips, UCD John O'Brien, TCD

Total Places	Core /Option
35	35

Module Description
This is a Postgraduate level course. Students are expected to have completed Undergraduate level prior learning. The module allows students to develop a theoretical, analytical and practical approach to the use of modern spectroscopic techniques for structure determination, namely Nuclear Magnetic Resonance (NMR) and mass spectrometry (MS). The physical principles underlying the spectroscopic methods will be outlined. Significant attention will be paid to instrumental factors that influence the outcome of NMR and MS experiments. The manner in which the spectroscopic methods can be brought together to solve structural problems will be presented and given as problem sets. Examples of applications from both organic and inorganic chemistry will be used.

Learning Outcomes
On successful completion of this module, students should: - Have a knowledge and understanding of the theoretical principles underpinning mass spectrometry and NMR spectroscopy. - Be familiar with the operational capabilities/constraints of each technique; - Be aware of the issues involved in sample preparation; - Be able to analyse and interpret data and have an appreciation of the limitations of each spectroscopic technique; - Be able to identify the most suitable spectroscopic techniques for the structure determination of a given sample. Course is graded as Pass (60%) or Distinction (76%)

Workload

Type	Hours
Specified Learning Activities	30
Lectures	18
Autonomous Student Learning	54
Total	**102**

Assessment Details

Description	Timing	Score By	% Final Grade
Based on Course Materials and Literature seaches x5	Varies	MRK	100
Total			**100**

Prior Learning

Type	Prior Learning
Recommended	Students are expected to have completed Undergraduate level prior learning of the basic principles of NMR Spectroscopy and Mass Spectrometry.

Module Remediation Strategies

Remediation
If you fail this module you may repeat or substitute where permissible. It is not possible to remediate this Module if the reason for failure is the non-submission or late submission of assignments.

CHEM40390 – Topics in Inorganic Chemistry

Short Title	Long Title
Topics in Inorganic Chemistry	Topics in Inorganic Chemistry

Level	Credits	Semester	Passing Grade	Module Coordinator
4	5.0	Year Long Module	DPF	Andrew Phillips (UCD) TBA Bob Baker (TCD)

Total Places	Core /Option
30	30

Module Description

This module covers extensively modern and frontier aspects of inorganic chemistry. The module is divided into three sections. Students will develop a solid foundation in the coordination chemistry and organometallic chemistry of the Lanthanoid and Actinide elements. A large emphasis is placed on understanding the fundamental differences in 4f and 5f chemistry. The second part of the course focuses on the application of main group elements in modern organic synthesis. This includes topics on alkali and earth alkali reagents, especially recent advances in chiral and regio-selective nucleophilic additions. Use of Lewis acid catalysis, Diels-Alder cyclizations, Friedel-Crafts and Reformatsky type reactions will also be examined in-depth. Other topics of interest include (but are not limited to) polymerization and main-group supported hydrogenation. The bioinorganic part of the course is aimed at giving a survey of the most exciting recent developments in this field, covering hydrogenases, photosynthesis, iron-sulfur clusters, nitrogenase, heme iron enzymes, multinuclear copper sites and metal transport and protein assembly. Model chemistry, highly sophisticated spectroscopy and the biotechnological use of enzymes will be discussed.

Learning Outcomes

On successful completion of this module, students should:

- Have developed an appreciation of the everyday uses for these elements and their compounds
- Gained an understanding of 'exotic' chemistry
- Be able to apply the taught concepts to new problems in contemporary organo-f-element chemistry
- Have developed knowledge of how main group elements can be applied to handle difficult problems in organic synthesis
- Be able to identify biological problems, learn about possible synthetic and analytical approaches to problem solving and experience the effectiveness of using a combination of methods.

Course is graded as Pass (60%) or Distinction (76%)

Workload

Type	Hours
Specified Learning Activities	30
Autonomous Student Learning	50
Lectures	18
Small Group	2
Tutorial	3
Total	**103**

Assessment Details

Description	Timing	Score By	% Final Grade	In Blackboard ?
Assignments x3	Varies	MRK	100	N
Total			**100**	

Module Remediation Strategies

Remediation
If you fail this module you may repeat or substitute where permissible. It is not possible to remediate this Module if the reason for failure is the non-submission or late submission of assignments.

CHEM40400 – Masterclass in Carbohydrate Chemistry

Short Title	Long Title
Masterclass in Carbohydrate Chem	Masterclass in Carbohydrate Chemistry

Level	Credits	Semester	Passing Grade	Module Coordinator
4	2.5	Semester One	DPF	Eoin Scanlan, TCD Stefan Oscarson, UCD

Total Places	Core /Option
20	20

Module Description

The carbohydrate module will provide students with an in-depth knowledge of recent advances in synthetic and biological carbohydrate chemistry. Topics will include: synthetic strategies towards oligosaccharides and glycoconjugates, the structure, function and physiological relevance of glycosylation, glycosensor development and protein modification. Lectures will be given by a number of leading experts in the field. Concepts introduced in the lectures will be further elaborated and discussed through a number of small-group workshops.

Learning Outcomes

* Gain an understanding of carbohydrate and glycosylation chemistry and mechanism
* Be able to design and critically assess a synthetic strategy for complex oligosaccharides and glycoconjugates
* Understand the biological relevance and therapeutic applications of carbohydrates.

Workload

Type	Hours
Lectures	15
Specified Learning Activities	20
Autonomous Student Learning	20
Total	**55**

Assessment Details

Description	Timing	Score By	% Final Grade	In Blackboard ?
< Description >	End_Sem_Sub	MRK	100	N
Total			**100**	

CHEM40450 – Surface Science and Technology

Short Title	Long Title
Surface Science & Tech (TCD)	Surface Science and Technology (TCD)

Level	Credits	Semester	Passing Grade	Module Coordinator
4	5.0	Semester One	DPF	Cormac McGuinness, School of Physics, TCD

Module Description
The module provides a detailed examination of all of the practical aspects of measurements on surfaces. It covers the fundamentals of vacuum creation and pressure measurement; the nature of surface structure and how it is determined; how surfaces are characterized; and how they are prepared for chemical processes.

Learning Outcomes
On completion of this module, students should be able to use various techniques to characterize a given surface including: low energy electron diffraction (LEED); reflection high energy electron diffraction (RHEED); photoelectron diffraction; x-ray photoelectron spectroscopy (XPS); electron spectroscopy for chemical analysis (ESCA); Auger electron spectroscopy (AES); scanning Auger microscopy (SAM); secondary ion mass spectrometry (SIMS) and various other mass spectrometric techniques; scanning tunneling microscopy (STM); atomic force microscopy.

Workload

Type	Hours
Specified Learning Activities	18
Lectures	18
Autonomous Student Learning	54
Total	**90**

Assessment Details

Description	Timing	Score By	% Final Grade	In Blackboard ?
	End_Sem_Exam_2	MRK	100	N
Total			**100**	

Prior Learning

Type	Prior Learning
Required	Basic undergraduate physics or chemistry

Module Remediation Strategies

Remediation
If you fail this module you may repeat, resit or substitute where permissible.

CHEM40720 – Scientific Writing and Publishing

Short Title	Long Title
Publish or Perish (TCD)	Scientific Writing and Publishing (TCD)

Level	Credits	Semester	Passing Grade	Module Coordinator
4	2.5	Semester Two	DPF	Mathias Senge, TCD

Total Places	Core /Option
30	30

Module Description

The module aims to give students an overview about current publication strategies, trends, assessments and problems. The course will outline different types of research communications, develop strategies for their presentation and describe the current publication trends. Assessment strategies for the qualitative evaluation of publications will be described and discussed in the context of applied research metrics using database analyses. Historical and current trends in research politics will be discussed and compared to changes in publication strategies. Selected examples from current and past research will be used to illustrate questions such as fraud, misconceptions, literature analysis and publication forms.
Content outline:
1 .Why is scientific publishing necessary?
2. History of scientific publishing
3. The scientific paper
4. Tips for writing a good paper
5. The scientific publishing process
6. Measuring impact: Bibliometric analysis of publications
7. The WWW and scientific publishing

Learning Outcomes

On successful completion of this module, students should:
* Have a knowledge and understanding of the scientific publication process;
* Be apply to analyse publications critically with regard to research metrics;
* Be able to critically analyse current publications;
* Have improved their own science reporting skills;
* Be capable of analysing research advances in an historical and bibliometric context

Workload

Type	Hours
Specified Learning Activities	15
Lectures	10
Autonomous Student Learning	15
Total	**40**

Assessment Details

Description	Timing	Score By	% Final Grade	In Blackboard ?
Written exam	End_Sem_Exam_1	LET	100	N
Total			**100**	

Prior Learning

Type	Prior Learning
Recommended	Prior publication experience, interest in an academic career
Required	Basic undergraduate biochemistry and chemistry

CHEM40850 – Transmission Electron Microscopy

Short Title	Long Title
Transmission Electron Microscopy	Introduction to Transmission Electron Microscopy

Level	Credits	Semester	Passing Grade	Module Coordinator
4	5.0	Semester Two	DPF	Valeria Nicolosi, Aleksey Shmeliov, TCD

Total Places	Core /Option
20	20

Module Description

In the world of Nanotechnology, Material Science and Life Science, transmission electron microscopy has become an essential tool to investigate materials and correlate structures to properties. This lecture series will provide grounding in the fundamental theory, operating principles and applications of the electron microscope.
In the lectures, the basic electron optics, basic principles of TEM imaging and diffraction, radiation damage and image recording and processing are introduced. In the practical sessions, participants will get hands-on experience with particular attention on demonstrating the meaning of some of the most fundamental concepts covered during the lecture course.

Learning Outcomes

- Basic notions of electron microscopy
- Interaction electron/matter
- Electron diffraction
- Different imagine modes in TEM
- Image interpretation

Workload

Type	Hours
Practical	12
Lectures	8
Autonomous Student Learning	54
Specified Learning Activities	12
Laboratories	12
Total	**98**

Assessment Details

Description	Timing	Score By	% Final Grade	In Blackboard ?
Written Examination	End_Sem_Exam_2	LET	100	N
Total			**100**	

Module Remediation Strategies

Remediation
If you fail this module you may repeat, resit or substitute where permissible

CHEM40860 – Chemistry Education and Public Engagement (EPE)

Short Title	Long Title
Chemistry EPE	Chemistry Education and Public Engagement (EPE)

Level	Credits	Semester	Passing Grade	Module Coordinators
4	5.0	Year Long Module	Fail/Pass/Merit/Distinction	John O'Donoghue, Niamh McGoldrick, Noelle Scully, Sylvia Draper

Total Places	Core/Option
16 (TCD PG only)	5

Module Description
The module aims to give students the opportunity to develop presentation and teaching skills in a real world setting. It introduces them to education and public engagement (EPE) theories and best practice. It provides them with the hands-on experience they will need to disseminate chemical principles and research concepts to younger audiences and the general public. It involves the delivery of presentations and/or demonstration workshops in schools as well as large scale public events. Discussions around the public perception and attitudes to Chemistry are examined in a group setting.

Learning Outcomes
On successful completion of this module, students should: • Have a knowledge and understanding of the public image of chemistry in popular media. • Have developed their own effective communication style. • Have developed and improved presentations and workshop ideas for different audiences. • Be in a position to design and implement demonstrations and workshops for schools and the public. • Be able to select and analyse hot topics within Chemistry. • Be able to explain their research area and to engage non-specialists. • Have learnt how to evaluate effective communication platforms through self-reflection and feedback. Course is Graded as Fail, Pass (50%), Merit (60%) or Distinction (70%)

Workload

Type	Hours
Specified Learning Activities	40
Lectures	5
Autonomous Student Learning	40
Class Discussion	20
Total	105

Assessment Details

Description	Timing	Score	% Final Grade	In Blackboard ?
Public or school based presentations/workshops and self-reflection journal	Thr_Sem	PFD	60	N
Group project and poster/presentation.	Thr_Sem	PFD	40	N
Total			100	

CHEM40910 – Quantitative Molecular Modelling

Short Title	Long Title
Quant Mol Modelling (TCD)	Quantitative Molecular Modelling (TCD)

Level	Credits	Semester	Passing Grade	Module Coordinator
4	5.0	Semester One	DPF	Graeme Watson, TCD

Total Places	Core /Option
35	35

Module Description

The module aims to give students an overview of the principles underlying the standard quantum mechanics techniques for simulation of the structure and properties of molecular systems. This will include the basic theory behind the approaches as well as practical aspects such as basis set choice. This course will include the performance of different approaches such HF, DFT, MP2, CI, CC

Learning Outcomes

On successful completion of this module, students should:

- Understand potential energy surfaces, important points, basic optimization and molecular dynamics. (3)
- Understand at a basic level the Hartree-Fock approach and its approximations (3)
- Know the definition of correlation, where it is important and the key aspects of post-HF approaches, including correlation (MP2, CI, MCSCF, CC) (3)
- Have a basic understanding of Density Functional Theory (LDA / GGA / Hybrid) and its differences compared to wavefunction approaches (i.e. Hartree-Fock) (3)
- Have a detailed knowledge of different types and the naming of basis sets including minimal, double /triple zeta, split-valence, polarisation and diffuse functions. (2)
- Be able to choose an appropriate method for a particular problem based on analysis of the performance of different approaches to different problems. (1)
- Prepare a Gaussian09 input file, include a basis set and methodology, and analyse the results (using Gaussian09 for Windows and Gaussview) (1)

Workload

Type	Hours
Practical	12
Autonomous Student Learning	54
Specified Learning Activities	12
Laboratories	12
Lectures	12
Total	**102**

Assessment Details

Description	Timing	Score By	% Final Grade	In Blackboard ?
5 Assignment Sheets	Thr_Sem	LET	30	N
Laboratory Work	Unspecified	LET	40	N
Written Paper	End_Sem_Exam_2	LET	30	N
Total			**100**	

Module Remediation Strategies

Remediation
If you fail this module you may repeat or substitute where permissible. It is not possible to remediate this Module if the reason for failure is the non-submission or late submission of assignments.

CHEM40920 – Translational Studies in HIV infections

Short Title	Long Title
Translational Research in Aids	Translational Research in Aids

Level	Credits	Semester	Passing Grade	Module Coordinator
4	2.5	Semester Two	DPF	Isabel Rozas, TCD

Total Places	Core /Option
30	30

Module Description
This module aims to give students an overview of the history and actual situation of the HIV pandemic known as AIDS and how this affects Ireland. Moreover, the virus cycle and possible targets and the therapies that have been and are being developed for each of these targets will be presented. Finally, a discussion on the advances made at a biochemistry level and with vaccines as well as an outline of how AIDS is dealt with in Dublin's hospitals will be offered.

Learning Outcomes
On successful completion of this module, students should: * Understand what AIDS is and how it affects the world * Understand how AIDS affects Ireland * Know the HIV life cycle and how this cycle offers different targets to kill the virus * Have a detailed knowledge of established therapies and new developments in drugs aimed at each of these targets * Have a basic understanding of biochemistry developments in the treatment of AIDS and of research on a possible vaccine * Understand how AIDS is being treated in a Dublin hospital

Workload

Type	Hours
Autonomous Student Learning	38
Lectures	12
Total	**50**

CHEM41300 – Mass Spectrometry for Chemical and Biochemical Research

CHEM41420 – Advanced Oxidation Processes

Short Title	Long Title
Advanced Oxidation Processes	Advanced Oxidation Processes

Level	Credits	Semester	Grade Scale	Module Coordinator
4 - Masters	2.5	Spring	Distinction/Pass/Fail (GPA Neutral)	Jhimli Paul Guin

Total Places	Core/Option
20	20

Module Description
Advanced oxidation processes have a wide range of environmental chemistry and advanced material preparation applications. These include water remediation using solar energy and preparation of polymeric materials for therapeutic purposes or for sustainable agriculture. The content of this module includes 1) fundamental difference between advanced and general oxidation processes, 2) different types of advanced oxidation processes including Fenton, ozonation, photocatalysis, electrochemical oxidation, high energy radiation (viz. electron beam and gamma radiation), 3) chemistry of in-situ production of reactive oxidising radicals and associated chemistry in aqueous and non-aqueous solvents. 4) use of oxidising radicals for polymer grafting and preparation of polymer nanocomposites, hydrogels, superabsorbent hydrogels, etc. 5) use of oxidising radicals for elimination of persistent organic compounds, endocrine disrupting chemicals, dyes and pharmaceutical compounds in ground and surface waters.

Learning Outcomes
On successful completion of this module, students should: • Recognize and classify different types of advanced oxidation processes. • Understand the mechanism of radical formation. • Understand the mechanisms of formation of grafted polymers superabsorbent hydrogels. • Understand the differing mechanisms of water de-pollution processes.

Workload	
Type (e.g. Lectures/Self-directed learning etc.)	**Hours**
Conversation Class	8
Lectures	8
Specified Learning Activities	10
Autonomous Student Learning	26
Total	**52**

Assessment Details			
Description	**Timing**	**Examiner**	**% of Final Grade**
An assignment submitted two weeks after the module's delivery	Throughout the Trimester	Jhimli Paul Guin	50
Classroom assignment and presentation on day 1	n/a	Jhimli Paul Guin	25
Classroom assessment and presentation during day 2	n/a	Jhimli Paul Guin	25
Total			100

Remediation
If you fail this module you may repeat or substitute where permissible. It is not possible to remediate this Module if the reason for failure is the non-submission or late submission of assignments.

CHEM50030 – Chemistry Third Year PhD Presentation*

Short Title	Long Title
Chem 3rd Yr PhD Presentation	Chemistry Third Year PhD Presentation

Level	Credits	Semester	Passing Grade	Module Coordinator
5	2.5	Semester Three	DPF	Declan Gilheany (UCD)

Total Places	Core /Option
60	60

Module Description

Third Year PhD students have to make an oral presentation of their research area and the results of their research. The presentation will be of the form of that given at a major international conference in their subject area. The audience will comprise their peers, academics from the Schools of Chemistry at UCD/TCD, invited representatives of funding agencies and interested industry participants.

Assessment is based mainly on the quality of the presentation rather than on the quality of the research results. Course is graded as Pass (60%) or Distinction (76%). There are usually also prizes for the best presentation.

Learning Outcomes

On completion of this module, students will have learned the steps necessary to make an effective presentation including: selection of material, outline of the story to be told, construction of slides (e.g. PowerPoint), location of the talk, method of delivery, nature of the audience, the obtaining of feedback.

Workload

Type	Hours
Specified Learning Activities	18
Autonomous Student Learning	18
Seminar	18
Total	**54**

Assessment Details

Description	Timing	Score By	% Final Grade	In Blackboard ?
Conformity to the Abstract Template	Unspecified	MRK	10	N
The Giving of the Seminar	End_Sem_Sub	MRK	30	N
The Quality of the Seminar	End_Sem_Sub	MRK	60	N
Total			**100**	