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Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

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

Contents

* Compulsory Module

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	Semester One and Two	PF	Yurii Gun'Ko, 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 reflection 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

CHEM40450 – Surface Science and Technology

Short Title	Long Title
Surface Science & Tech	Surface Science and Technology

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	Scientific Writing and Publishing

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, 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 – Science Communication

Short Title	Long Title
Science Communication (SciComm)	Science Communication, 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 science PhD students the opportunity to develop presentation, communication, and teaching skills in real-world settings. Through training workshops, it introduces them to established education and public engagement (EPE) theories and best practice in Science Communication. A specific emphasis is placed on the public perception and attitudes to Chemistry, looking at the duality of the discipline which sets it apart from other areas of science. The module provides students with the hands-on experience they need to disseminate scientific principles and research concepts to younger audiences and the general public. The required work experience involves the delivery of presentations, talks and/or demonstration workshops in schools as well as public events.

Learning Outcomes
On successful completion of this module, students should: Have a knowledge and understanding of the public image of science, particularly 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 from their own area of expertise. Be able to explain their research area and to engage non-specialists. Have learnt how to evaluate effective communication through self-reflection and feedback. Course is Graded as Fail, Pass (50%), Merit (60%) or Distinction (80%)

Workload

Type	Hours
Specified Learning Activities	30
Lectures/workshops	5
Autonomous Student Learning	40
Discussion and Group Work	30
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 (MS Teams)
Group project and poster/presentation.	Thr_Sem	PFD	40	N (MS Teams)
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.

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**	