UNIVERSITY COLLEGE LONDON

DEPARTMENT OF CHEMISTRY

Centre for Doctoral Training in Molecular Modelling and Materials Science

COURSE HANDBOOK

Mres in Molecular Modelling & Materials Science

MSc in Molecular Modelling
SESSION 2016/2017
Dates of College Terms 2016/2017

First Term    Monday 26 September 2016 – Friday 16 December 2016 (12 weeks)
Second Term  Monday 09 January 2017 - Friday 24 March 2017 (11 weeks)
Third Term    Monday 24 April 2017 - Friday 09 June 2017 (7 weeks)

However, please note that both courses run for a whole year (September – September).
While every effort has been made to ensure the accuracy of the information in this document, the CDT cannot accept responsibility for any errors or omissions contained herein.
Calendar 2016-2017

Monday 26 September  Welcome session (room 319 of Chemistry)

Monday 3 October  CHEMGM04 (room 319 of Chemistry)
and other Lectures for first term courses

25 November  CHEMGM04 Simulation Project Poster session
(Nyholm room of Chemistry)

Wednesday 11 January  CHEMGM04 examination (room 319 of Chemistry)

Tuesday 28 February  Deadline for submission Literature Review report-CHEMGM02

May/June  Examinations of Lecture Courses

Friday 25 August  Deadline for submission research project report
(CHEMGM01/CHEMGM99)

5-16 September  Oral presentations and viva voce examinations
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1. Introduction

The aim of this Handbook is to provide you with a range of useful information related to your life as a student at University College London. It complements the College and the department Student Handbooks, which should be provided to you on admission.

2. General information

2.1 Contacts of members of the M3S CDT’s staff

Members of both teaching & administration staff of the CDT can be contacted by e-mail, phone or the internal mail service. Mail boxes (pigeon holes) for staff are situated on ground floor of Department of Chemistry.

<table>
<thead>
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<th>Role</th>
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</table>

2.2 Attendance

Students are obliged to attend the lectures and their research project regularly. If you are unable to do so for any reason, you should inform the manager of the M3S CDT, Dr Zhimei Du (Tel: 02076797465, email z.du@ucl.ac.uk), or your supervisor as soon as possible. This should be done either in person, by telephone, letter (internal mail or normal mail) or email.
For extended absence due to illness, you must provide a Medical Certificate upon your return to College.

Students will be expected to schedule their project work in conjunction with their project supervisor. Remember that the project counts for 50% for MSc and 58% for MRes. Hence, steady work throughout the year will be necessary.

3. MRes in Molecular Modelling and Materials Science course structure

The programme provides specific training in molecular modelling methods and structure determination and characterisation techniques applicable to the materials sciences, together with tuition in research methods and the use of literature sources. The taught courses cover both specialist scientific topics and professional skills training relevant to the industrial environment.

The MRes course Molecular Modelling and Materials Science contains a number of independent modules, assessed separately by coursework, examination or a mixture of both.

Course Requirements

5 course units = 180 credits ≈ 1800 hrs of study
20 “Roberts” points requested for EPSRC funded students

Participation in Centre Activities

Core modules:
- CHEMGM04 Simulation Methods in Materials Chemistry 30 credits
- CHEMGM02 The Scientific Literature 15 credits

Optional Modules (After consultation with your research supervisor select either two of the following optional modules OR one of the optional modules and an elective module)
- EDUCGE02 Researcher Professional Development 15 credits
- CHEMGG90 Transferable Skills for Chemists 15 credits
- MSING002 Mastering Entrepreneurship 15 credits
- CHEMGM03 Simulation Methods in Materials Chemistry (only for those who need to take English language course) 15 credits
Elective modules
Choice of one UCL postgraduate lecture course worth 15 credits

Dissertation/report
CHEMGM01 Advanced Research Project 105 credits

Activities
Seminars, CDT’s annual Industry Presentation Day.

Award scheme
In order to award the certificate, the student must complete 5 course units and gain 180 credits and pass all components at a level of 50% or better. For a merit award, students have to achieve an overall mark of 60 with minimum of 60 in his/her research project. For a distinction award, an overall mark of 70 together with 70 in the research project is required.

If a student passes a module at resit stage, his/her degree shall not be awarded with merit or distinction.

For automatic progression from MRes to MPhil/PhD or EngD, a student needs to achieve an average mark of no less than 60% in the independent, original research components and no less than 50% in the taught elements.

In cases where a student did not meet these requirements, but who has the support of the MPhil/PhD or EngD programme organisers, a case in writing can be made to the Chair of the Research Degree Committee for the consideration of suspension of regulations. For more details, please read (http://www.ucl.ac.uk/srs/academic-regulations/docs/mres.pdf).

4. MSc in Molecular Modelling course structure
Students will gain detailed knowledge and skills in molecular modelling, focusing on the state-of-the art simulation techniques employed to research the molecular level properties that determine the macroscopic behaviour of matter. They will also gain key research skills and will learn the basic concepts in business and entrepreneurship as applied to high tech industries.
The programme is delivered through a combination of lectures, seminars and laboratory classes. Assessment is through unseen examination, coursework, individual and group projects, poster creation, presentation and the research project.

Course Requirements

Students undertake modules to the value of 180 credits. The programme consists of two core modules (45 credits), three optional/elective modules (45 credits) and a research project (90 credits).

In addition, the students are requested to participation in Centre Activities.

Compulsory modules:

- CHEMGM04 Simulation Methods in Materials Chemistry 30 credits
- CHEMGM02 The Scientific Literature 15 credits

Optional Modules (After consultation with your research supervisor select either two of the following optional modules and an elective module OR one of the optional modules and two elective modules)

- EDUCGE02 Researcher Professional Development 15 credits
- CHEMGG90 Transferable Skills for Chemists 15 credits
- MSING002 Mastering Entrepreneurship 15 credits
- CHEMGM03 Simulation Methods in Materials Chemistry (only for those who need to take English language course) 15 credits
- CHEMGG44 Numerical Methods in Chemistry 15 credits

Elective modules

Choice of one UCL postgraduate lecture course worth 15 credits

Dissertation/report

CHEMGM99 Computational Research Project 90 credits
Activities
Seminars, CDT's annual Industry day.

Award Scheme
In order to award the certificate, a student must complete 6 course units and gain 180 credits and pass all components at a level of 50% or better. For a merit award, students have to achieve an overall mark of 60 with minimum of 60 in his/her research project. For a distinction award, an overall mark of 70 together with 70 in the research project is required.

If a student passes a module at resit stage, his/her degree shall not be awarded with merit or distinction.

5. A short description of each module

5.1 CHEMGM04 Simulation Methods in Materials Chemistry
This is an intensive 30-lecture course taught over five weeks. The course will discuss the background to computer modelling techniques used in materials simulations, including Interatomic Potential-based Methods (Energy Minimisation, Molecular Dynamics, Monte Carlo), Ab initio methods (Hartree Fock, Density Functional Theory) and properties that we can obtain from simulations.

Lectures are held on Mondays, Tuesdays and Thursdays 9-11 am for five weeks, starting on Monday 3rd October 2016.

5.1.1 Simulation Project
In tandem with the CHEMGM04 lecture course, the students will carry out a Simulation Project, which reinforces the taught subjects through hands-on simulations.

Supervised lab classes are held on Mondays-Thursdays 2-5 pm for five weeks, starting on Monday 3rd October 2016.

Assessment is by coursework and a group poster essay.

Assessment of this module: coursework (30%), poster (10%) and 2.5 hours written examination (60%)
5.2 CHEMGM02 The Scientific Literature

The literature project provides the student with the opportunity to learn how to use the Scientific Literature, both in the print and electronic database forms, to discover what is known about a particular topic, and write a "state-of-the-art" review. You will be expected to find the relevant scientific papers, using tools such as the Science Citation Index and Beilstein, to abstract the important and relevant information from the papers, and to formulate and condense this material into a review which is of value to others.

The review should be approximately 5,000 to 7,000 words and no more than 25 pages should be word-processed in Times New Roman, 12 pt font, 1.5 spaced, and should contain at least 30 substantive references. The word/page limit for the literature review excludes the contents page, reference list etc. Reports should be bound so that they are not bulky and can lie flat when open, for example plastic comb-binders. Two copies of the report need to be submitted.

5.3 EDUCGE02 Researcher Professional Development

The module aims to:

- develop participants’ conceptions of what it means to be a professional;
- develop participants’ understanding of how professional development occurs;
- develop participants’ ability to forward their own professional development;
- develop participants’ abilities to learn from experience with planning, action & reflection.

- By the end of the component, participants should be able to:
  - understand the meanings of professionalism and professional development;
  - know about professional development methods;
  - know how to plan and manage their own professional development and support others;
  - critically evaluate professional development needs and progress claimed, in an evidence-based case.

All teaching sessions will be held on Fridays, except individual meetings, which will be scheduled with the participants for the days shown.
5.4 CHEMGG90 Transferable Skills for Chemists

The module contains two distinct sections, one on presentation of information via multiple mediums and a second part which provides choice of a selection of individual skills modules.

For the presentation sub-component students will work in groups to investigate an assigned research topic and select five papers that best describe the topic they are assigned. Together they will prepare and deliver an oral presentation describing the research topic, referencing the chemical literature. They will also prepare and present a poster on the same topic. This component aims are to teach students how to critically select appropriate scientific papers and how to disseminate the relevant details to different audiences.

The individual skills modules will focus on ancillary skills many Chemistry practitioners require including retrieval of information from databases, use of specialist software packages and analysis and presentation of data. These will mostly be delivered via self-study course content presented and assessed electronically, although there will be one general laboratory skills module also. Students will select two of these sub-components (40 learning hours each, including time directly on task and additional reading).

5.5 MSING002 Mastering Entrepreneurship

Aims

This course will be of interest to those who are considering creating their own business or who envisage having a role promoting new initiatives within an existing business organisation. The aim of the course is to give an understanding of:

• the criteria for success of a new business - personal, market & technical
• business planning and securing the necessary resources - including finance - for the new business

The course will draw heavily for illustration and illumination on a range of case studies mostly from high-technology ventures. These fascinating case studies best illustrate the challenges of creating high potential enterprises

Objectives
By the end of the course students should:

- have a clearer view of how to judge the potential of a high-potential business concept
- understand the difference between a true opportunity and just another idea
- recognise the effort and dedication needed to make a business succeed
- be aware of the different marketing challenges faced by ‘breakthrough’ products and ‘me-too’ products
- recognise the importance of direct experience in an industry and of reputation and existing relationships with others in the industry
- have an understanding of the various sources of finance (conventional and unconventional) and to know how to make a case to financial investors

5.6 CHEMGG44 Numerical Methods in Chemistry

Aims

To introduce scientific mathematical analysis in a single-course and to inspire the use of mathematical solutions in scientific analysis.

Approximately 10 tests taken as the course progresses

5.7 Postgraduate Lecture Course

Choice of one postgraduate 15 credit lecture course in any Department in UCL. Students are advised to consult with their research supervisor, before deciding on the course choice.

5.8 CHEMGM99 Computational Research Project

The Research Project Report should detail the research carried out, introducing the topic and its relevance, explaining the methodology and discussing the research findings in relation to the existing literature. Assessment of the Research Report will be based primarily on the science presented and the indications given of the scientific knowledge and research capabilities of the student. The quality of English and presentation will also be taken into account. For various reasons it occasionally turns out that a research project leads to very few new results but a well-written report with good scientific content will still lead to a high mark. The report should be approximately 10,000 to 12,000 words. The word limit excludes the contents page, reference list etc. The report should be word-processed in Times New Roman,
Assessment of the research project is through (i) a report from the academic Research Supervisor (30%). (ii) The Project Report (30%), which will be assessed independently by two examiners from the Centre’s academic committee, one who will be the specialist topic examiner and another who may not be expert in the specialist research area (general examiner). (iii) an Oral presentation (10%). The presentations will be scheduled together as a mini-symposium in September and (iv) a viva voce examination (30%).

5.9 CHEMGM01 Advanced Research Project

The Research Project Report should detail the research carried out, introducing the topic and its relevance, explaining the methodology and discussing the research findings in relation to the existing literature. Assessment of the Research Report will be based primarily on the science presented and the indications given of the scientific knowledge and research capabilities of the student. The quality of English and presentation will also be taken into account. For various reasons it occasionally turns out that a research project leads to very few new results but a well-written report with good scientific content will still lead to a high mark.

The report should be approximately 12,000 to 15,000 words. The word limit excludes the contents page, reference list etc. The report should be word-processed in Times New Roman, 12 pt font, 1.5 spaced. In addition (and if appropriate), supplementary material (spectra, tables, software programs, etc.) should be included as appendices to ensure completeness but examiners are not obliged to read this extra material. However, examiners will want to see the evidence, such as representative NMR spectra, upon which conclusions are based. Reports should be bound so that they are not bulky and can lie flat when open, for example plastic comb-binders. Two copies need to be submitted.
Assessment of the research project is through (i) a report from the academic Research Supervisor (30%). (ii) The Project Report (30%), which will be assessed independently by two examiners from the Centre’s academic committee, one who will be the specialist topic examiner and another who may not be expert in the specialist research area (general examiner). (iii) An oral presentation (10%). The presentations will be scheduled together as a mini-symposium in September and (iv) a viva voce examination (30%).

6. Penalties for Late Submission of Coursework
   i) The full allocated mark will be reduced by five percentage points for the first working day after the deadline for the submission of the coursework.
   ii) The mark will be reduced by a further ten percentage points if the coursework is submitted during the following six days.
   iii) Providing the coursework is submitted by a date during term three defined in advance by the relevant Master’s Board of Examiners, but had not been submitted within seven days of the deadline for the submission of the coursework, it will be recorded as zero but the assessment would be considered to be complete
   iv) In the case of dissertations and project reports submitted more than seven days late, the mark will be recorded as zero but the assessment would be considered to be complete.
   v) Where there are extenuating circumstances that have been recognised by the Board of Examiners or its representative, these penalties will not apply until the agreed extension period has been exceeded.

7. Penalties for Over-length Coursework, including Research Projects, Dissertations and Final Reports
For submitted coursework, where a maximum word count has been specified, the following procedure will apply:
   i) Assessed work should not exceed the prescribed word count.
   ii) Assessed work with a stated word count above the prescribed word count should not be accepted for submission (i.e. it will not be date-stamped or otherwise recorded as formally submitted), but immediately returned to the student with instructions to reduce the word length. The work may then be resubmitted but the original deadline for submission still applies and penalties for late submission will be applied.
iii) For work that exceeds the upper word limit by 10% or more, a mark of zero will be recorded.

iv) For work that exceeds the upper word limit by less than 10% the mark will be reduced by ten percentage marks; but the penalised mark will not be reduced below the pass mark, assuming the work merited a pass.

v) For discipline specific practices such as bibliographies, tables, pictures and graphs, departments/divisions should specify in writing to students whether these are recorded as part of the upper word limit and how this will be counted.

8. Plagiarism prevention and detection

The presenting of other peoples’ work as your own work is a very serious offence known as Plagiarism. Plagiarism is taken extremely seriously by the Department and by UCL, as well as in the academic and publishing world at large. If a student is found to have committed plagiarism, it can lead to the student not being awarded a degree, and being excluded from all future examinations at UCL and/or the University of London.

To understand what plagiarism is and how to avoid it please go to:

http://www.ucl.ac.uk/current-students/guidelines/plagiarism

All written reports may be checked for plagiarism using software Turnitin®, which is provided to UK universities by JISC.