

MPLS Divisional Board

Approved by the Director of Studies and the MSc Course Director in September 2023.

Title of Programme

MSc Theoretical and Computational Chemistry

Brief note about nature of change:

1. Minor wording changes

Location of change

In *Examination Regulations 2023/2024*:

<https://examregs.admin.ox.ac.uk/Regulation?code=moscitandcompchem>

Effective date

For students starting from MT 2024

For first examination from 2024/2025

Detail of change

Amend citation reference 1.1-1.21 as follows (new text underlined, deleted text struck through):

- ^{1.1}1. An Organising Committee shall be appointed which shall have power to arrange lectures and other instruction.
- ^{1.2}2. Candidates shall follow for at least three terms a course of instruction in Theoretical and Computational Chemistry, as determined by the course timetable.
- ^{1.3}3. The examination shall be in two parts, as follows:
 - ^{1.4}(a) Candidates shall successfully complete the prescribed coursework and/or tests on each of the taught modules offered, as specified below.
 - ^{1.5}(b) Candidates shall submit a project report on a project selected by the candidate in consultation with the supervisor, and approved by the

organising committee. The project report shall be assessed by the supervisor and one other academic appointed by the organising committee.

- ~~1.6~~ 4. The Director of the Centre for Doctoral Training in Theory and Modelling in Chemical Sciences or an appointed deputy shall make available to the examiners a certificate showing the extent to which the candidate has an adequate command of the topics in the modules offered and the assessment of the project.
- 1.7 5.4. The nature of the assessed work for each module will depend on the nature of the module and will be specified in the course handbook. Completed assignments must be submitted in accordance with the instructions and by the deadlines specified in the course handbook.
- 1.8 6.5. Assessed work for any failed module may be resubmitted before noon on 1st September for consideration by the board of examiners.
- 1.9 7.6. A candidate who has failed to satisfy the examiners may enter again for the examination on one, but not more than one, subsequent occasion, not later than one year after the initial attempt, and need only resubmit the assessed work for failed modules.
- 1.10 8.7. Candidates may be examined viva voce at the Examiners' discretion.
- 8. The list of taught modules will be published in the Course Handbook.

~~1.11~~ *List of taught modules*

- ~~1.12~~ 9. Candidates are required to take the following eight core modules:-
- ~~1.13~~ Quantum Mechanics-
- ~~1.14~~ Statistical Mechanics-
- ~~1.15~~ Mathematics 1-
- ~~1.16~~ Statistics-
- ~~1.17~~ Introduction to Programming-
- ~~1.18~~ Methods of Computer Simulation-
- ~~1.19~~ Electronic Structure Theory-
- ~~1.20~~ Software Development
- ~~1.21~~ 10. Candidates must take five option modules taken from the list below. Not all option modules will be available every year.-
- ~~1.22~~ Applied Computational Chemistry-
- ~~1.23~~ Biomolecular Simulation-
- ~~1.24~~ Mathematics 2-
- ~~1.25~~ Quantum Mechanics in Condensed Phases-
- ~~1.26~~ Intermolecular Potentials-
- ~~1.27~~ Chemical Informatics-
- ~~1.28~~ Chemical Reaction Dynamics-
- ~~1.29~~ Advanced Statistical Mechanics-
- ~~1.30~~ Advanced Quantum Mechanics-
- 1.31 Any other approved option module(s)

Explanatory Notes

Reference to the CDT in Theory and Modelling is to be removed as this CDT has closed. List of modules to be removed and students directed towards Course Handbook.