Master of Science by Coursework in Theoretical and Computational Chemistry

Brief note about nature of change:
This is to update the Examination Regulations to bring in line with the existing course structure. There are no changes to the assessment structure.

Location of change
2021-22, Master of Science by Coursework in Theoretical and Computational Chemistry (ox.ac.uk)

Effective date
For first examination from 2021

Detail of change

1.1. An Organising Committee shall be appointed which shall have power to arrange lectures and other instruction.

1.2. 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. The following routes shall be available:

14(a) M.Sc. in Theory and Computational Chemistry with progression to Probationer Research Student Status at the University of Oxford for a maximum of a further three terms in the Centre for Doctoral Training in Theory and Modelling in Chemical Sciences;
1.5 (b) M.Sc. in Theory and Computational Chemistry with progression to doctoral study at a partner institution in the Centre for Doctoral Training in Theory and Modelling in Chemical Sciences;

1.6 (c) M.Sc. in Theory and Computational Chemistry with no further progression to doctoral study at Oxford or with partner universities in the Centre for Doctoral Training in Theory and Modelling in Chemical Sciences.

1.7 3. The examination shall be in two parts, as follows:

1.8 (a) Candidates shall successfully complete the prescribed coursework and/or tests on each of the taught modules offered, as specified below.

1.9 (b) Candidates shall submit a project report on each of two short projects a project selected by the candidate in consultation with the supervisor, and approved by the organising committee. One of these projects shall be at Oxford and the other at one of the other partner institutions. The project report shall be assessed by the supervisor and one other academic appointed by the organising committee.

1.10 5.4. 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 assessments assessment of the two short projects project.

1.11 6.5. 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 assignments must be submitted, via the Administrator for the Centre for Doctoral Training in Theory and Modelling in Chemical Sciences, by the corresponding deadline specified in the course handbook. Completed assignments assignments must be submitted in accordance with the instructions and by the deadlines specified in the course handbook.

1.12 7. Any candidate who has failed four or more modules of any type at the first attempt will not be permitted to progress to the second year of the doctoral programme in the Centre for Doctoral Training in Theory and Modelling in Chemical Sciences.

1.13 8.6. Assessed work for any failed module may be resubmitted before noon on 1st September for consideration by the board of examiners.

1.14 9.7. 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. Such candidates will not be permitted to progress to the second year of the doctoral training programme in the Centre for Doctoral Training in Theory and Modelling in Chemical Sciences.

1.15 10.8. Candidates may be examined viva voce at the Examiners’ discretion.
1.16. The examiners may award a distinction for excellence in the whole examination.

1.17. The Director of the Centre for Doctoral Training in Theory and Modelling in Chemical Sciences or an appointed deputy shall have power to delete courses and to add other lecture courses to this list, and shall publish full details of any such changes in the University Gazette by not later than the Friday of the eighth week of the Trinity Term in the year preceding the examination.

1.18. The organising committee shall decide to which of the participating universities the student will transfer for their doctoral project in the second year, based on consultation with students and prospective doctoral supervisors, together if required with the results of the M.Sc.

1.19. List of taught modules

1.20. The following eight modules shall be designated core courses and must be offered by all candidates: Quantum Mechanics, Statistical Mechanics, Mathematics 1, Statistics, Computer Programming and Numerical Methods, Methods of Computer Simulation, Electronic Structure Theory, Software Development Training.

Candidates are required to take the following eight core modules:

- Quantum Mechanics
- Statistical Mechanics
- Mathematics 1
- Statistics
- Introduction to Programming
- Methods of Computer Simulation
- Electronic Structure Theory
- Software Development

1.21. The following nine modules shall be designated option courses and candidates must offer five of these for assessment: Applied Computational Chemistry, Biomolecular Simulation, Mathematics 2, Quantum Mechanics in Condensed Phases, Intermolecular Potentials, Chemical Informatics, Chemical Reaction Dynamics, Advanced Statistical Mechanics, Advanced Quantum Mechanics.

Candidates must take five option modules taken from the list below. Not all option modules will be available every year.

- Applied Computational Chemistry
- Biomolecular Simulation
- Mathematics 2
- Quantum Mechanics in Condensed Phases
- Intermolecular Potentials
- Chemical Informatics
- Chemical Reaction Dynamics
- Advanced Statistical Mechanics
• Advanced Quantum Mechanics
• Any other approved option module(s)

Explanatory Notes

This amendment is to reflect how the course is delivered now that it is no longer connected to a DTC and to correct the error that the regulations do not appear to have accurately reflected the stand-alone version of this course for some time.