**PROGRAMME SPECIFICATION FOR MSc IN THEORETICAL CHEMISTRY**

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| **1. Awarding institution/body** | **University of Oxford** |
| **2. Teaching institution** | **University of Oxford** |
| **3. Programme accredited by** | **n/a** |
| **4. Final award** | **M.Sc.** |
| **5. Programme** | **Theoretical Chemistry** |
| **6. UCAS code** | **n/a** |
| **7. Relevant subject benchmark statement** | **n/a** |
| **8. Date of programme specification** | **23.10.08** |

## 9. Educational aims of the programme

The aims of the programme are

- to introduce students to a wide range of theoretical topics and techniques in theoretical chemistry
- to develop mathematical skills and conceptual foundations as a preparation for research in a rapidly evolving environment
- to enable students to carry out directed research on a chemical topic involving theoretical development, and/or computational implementation, and to write a research report.

**10. Programme outcomes**

The purpose of the course is to provide a foundation in the concepts, methods and computational techniques of theoretical chemistry as a preparation for research. Training is also given in guided reading and directed research.

***A. Students will develop a knowledge and understanding of: new mathematical techniques, concepts and applications of quantum mechanics, statistical mechanics, molecular electronic structure and many-body theory. Students will also gain facility and experience in the use of computational packages and conducting directed research.***

*Related teaching/learning methods and strategies*

- Lectures in the mathematical techniques of complex analysis, vector algebra and special functions, with supporting problem classes to provide confidence and practice in new techniques.
- Lectures in quantum mechanics, statistical mechanics, molecular electronic structure and many-body theory, supported where appropriate by tutorials and guided reading to introduce new concepts and theoretical methods.
- Computational exercises will enable students to understand standard quantum chemistry computing packages and to apply them to problems in molecular electronic structure.
- The dissertation enables students to undertake an in depth study of a research problem involving theoretical understanding and/or computational modelling. Students are also trained in directed research, report writing, presentation and communication of results.
- Students are encouraged to follow recent developments by attending theoretical group seminars by internal and external invited speakers at least four times per term.

*Methods of Assessment*

Formative assessment will be provided for tutorial work and problem class work, as well as close supervision of the directed research project.

Summative assessment will be provided by:

- Term papers, set by the lecturers in mathematics (two papers) and moderated by the examiners, are designed to test understanding and problem solving skills.
- Assessed problem sets in Statistical Mechanics and Many Body Theory are graded by the lecturers.
- Extended essays, set by the lecturers in quantum mechanics, and moderated by the examiners, test the candidate's understanding, writing skills and use of library resources.
- The dissertation and oral examination, which are assessed by all examiners, test the candidate's ability to undertake directed research, to master the theoretical background and write a scientific report.

***B. Skills and other attributes***

***Students will have the opportunity to develop the following skills during the course:***

***I. Intellectual skills***

At the end of the course students will be expected to:

- analyse mathematical and scientific problems and to think logically.
- be able to undertake directed research in theoretical chemistry
- be able to give critical evaluation of reports and papers in theoretical chemistry

*Teaching/learning methods and strategies*

Problem classes, group discussion, extended essays, dissertation

*Assessment*:

As above.

II. ***Practical skill***s ***(where relevant)***

At the end of the course students will be expected

- to have improved their mathematical skills to a level broader and beyond that required for a particular research specialism.
- to carry out computational tasks in theoretical chemistry
- to be able to write research reports

*Teaching/learning methods and strategies*

Problem classes, computational exercises, dissertation.

*Assessment*

As above.

***III. Transferable skills***

Transferable skills include

- Critical analysis and logical evaluation of results.
- Construction of a logical argument.
- Initiative and imaginative use of techniques for problem solving.
- Time management.
- Preparation and presentation of research reports.
- Information handling, use of library and electronic resources.
- Written and oral communication.

*Teaching/learning methods and strategies*

Problem classes, tutorials, extended essays, dissertation.

*Assessment*:

As above

**11. Programme Structures and Features**

- Seven lecture courses with associated problem classes and directed reading.
- Extended essays are set over the Christmas and Easter vacations.
- Computational exercises.
- Dissertation. Students are required to submit a dissertation on a project in theoretical chemistry with a supervisor approved by the Chairman of Examiners. The dissertation is expected to give evidence that the candidate has read the background literature, performed directed research on a topic of current interest and properly assessed the value and significance of the results. This work constitutes 2-3 months work over the summer. Each candidate has an oral examination.

***Learning***

***This is a one year course comprising the following subjects, which are subject to annual review..***

**1. Vector calculus and special functions** (12 hours)
- Scalar and Vector Fields
- Line and surface integrals
- Gauss', Stoke's and Green's Theorems
- Curvilinear coordinates
- Series solutions of differential equations
- Bessel, Legendre and Hermite polynomials. Generating functions and recurrence relations.

**2. Complex analysis** (12 hours)
- Analytical functions. Cauchy's theorem. Poles and residues. Contour integration. Physical examples.
- Fourier and Laplace transforms.
- Green functions and simple integral equations.

**3. Quantum mechanics** (16 hours)
- Unitary operators and unitary transformations. Time evolution operator.
- Picture transformations. Schrodinger picture. Heisenberg picture and equation of motion. Dirac/interaction picture.
- Time dependent perturbation theory. The Dyson series.
- Density operator. Pure states. Statistical mixture of states. Applications.
- Second quantization. Harmonic oscillator: ladder method of solution, Creation/annihilation operators. Time development.
- Canonical quantization. The electromagnetic field.

**4. Statistical mechanics** (12 hours)
- Canonical, grand canonical and microcanonical ensembles; Fluctuations.
- Ideal quantum gases. Fermi gas and electrons in metals; Bose gas and Bose-Einstein condensation.
- Phenomenology of continuous phase transitions. Critical exponents, universality, scaling. Correlation functions. Examples.
- Statistical mechanical models: including Ising, lattice gas, XY, and Heisenberg; Solution of the one-dimensional Ising model.
- Mean-field theory, and its limitations.
- Renormalization group (real space).
- Aspects of classical imperfect gases.

**5. Molecular quantum mechanics** (8 hours)
- Many electron wavefunctions. Hartree products and Slater determinants. Second quantization
- Hartree-Fock approximations. Koopman's theorem. Brillouin's theorem. Restricted and unrestricted
- Hartree-Fock methods
- Configuration interaction

**6. Applied statistical mechanics** (8 hours)
- Focusing on a range of applications of Statistical Mechanics, including modern computational techniques.

**7. Many body theory (8 hours)**
- Second quantization. Canonical transformations. Models.
- Many-body Green functions (T=0), time-ordered; retarded/advanced,
- Non-interacting electrons. Metals and insulators. Feenberg series. Diagrammatics, renormalizations. Bethe lattices.
- Hubbard model. Mean-field approximation, unrestricted Hartree-Fock.

**12. Support for Students and their learning**

1. *Laboratory facilities* Students are allocated a desk in one of the research groups, with its own computer terminal.

2. *IT facilities* Access is open at all times to the departmental IT network, and extensive software, which are supported by two departmental IT staff. Network links to the good IT resources at colleges allow overnight access to the departmental facilities.

3. *Advice on course content/options* is available from the course director.

4. *Advice on research project* is available from the supervisor.

5. *Library facilities:* Internet access to all relevant recent journals is available. Books and older journal issues are available in the university science library within a five minute walk.

6. *Pastoral care*: in the event of difficulty, support is available in the student's College, from the project supervisor, the course director and the director of studies.

**13. Criteria for Admission**

- Applications are made to the faculty/department and then subsequently to colleges in the case of graduate students.

- The University regards as an overriding priority the admission of suitably-qualified candidates well-matched to their chosen course. It seeks to select graduate students solely on the grounds of proven and potential academic excellence, and its admission procedures are geared to this end.

- Candidates for admission to the MSc in Theoretical Chemistry will be expected to have qualifications equivalent to a first class or good upper second class degree in chemistry, physics or materials science, with particular emphasis on their mastery of mathematics, quantum mechanics and statistical mechanics.

- Prospective colleges check whether the applicant has adequate financial support.

- Applicants are chosen on academic merit, their referee's reports and their motivation.

**14. Methods for evaluating and improving the quality and standards of learning**

**Methods of evaluating and improving standards include:**

- The external examiner system (including moderation of students' assessed work).
- Review of examiners reports and student performance
- Student feedback
- Content approved by the Academic Committee of the Chemistry Department
- Periodical review by the MPLS Division.

**15. Regulation of assessment**

- Responsible bodies are responsible for establishing and approving any changes to examining conventions for the courses under their control. Responsible bodies also nominate the internal and external examiners on the Examination Boards for each of their degree courses, subject to approval by the Vice-Chancellor and Proctors on behalf of the University.
- Boards of Examiners, under their elected Chairs, are responsible for setting all papers, and marking the scripts of the examinees. They may appoint Assessors to assist in the setting and marking of the more specialist papers. After scripts have been marked, the Board of Examiners meets to classify the students in accordance with the rules established by the Examinations Committee.
- External Examiners are appointed in order:

  To verify that standards are appropriate to the award, in part by comparison with the standards of comparable institutions, and to ensure that the assessment procedures and the regulations governing them are fair and otherwise appropriate.

  To ensure that the conduct of the examination and the determination of awards has been fairly conducted, and that individual student performance has been judged in accordance with the regulations and conventions of the Examining Board. This will entail signing the Class List as an endorsement that the processes of examination and classification have been fairly conducted.
- External Examiners are expected to report to the Vice-Chancellor in each year in which they act. Their reports are expected to cover all the following points:
- the standards demonstrated by the students
- the extent to which standards are appropriate for the award
- the design, structure and marking is assessments
- the procedures for assessment and examinations
- whether or not external examiners have had sufficient access to, and the power to call upon, any material necessary to make the required judgements
- students' performance in relation to their peers in comparable courses
- the coherence of the policies and procedures relating to external examiners and their consonance with the explicit roles required of them
- the basis and rationale for any comparisons made
- the strengths and weaknesses of the students as a cohort
- the quality of teaching and learning which may be indicated by student performance
- The report is addressed to the Vice-Chancellor, and will be considered by the relevant divisional board, the faculty/department and by the University's Educational Policy and Standards Committee.
- Where an external examiner's report contains particular suggestions or criticisms, it is the responsibility of the faculty/department to ensure that full consideration is given to these, to institute further discussion or action, and to inform the external examiner within a reasonable time of what is done.

**Marking Scale**

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| **A+** | | Outstanding – the student's assignment was excellent and was moreover of outstanding quality at the MSc level. Distinction is awarded at this level. |
| **A** | | Excellent – the student has demonstrated an excellent understanding of almost all of the material, and has completed almost all of the assignment satisfactorily. |
| **A-** | | Very good – the student has demonstrated a very good understanding of most of the material, and has completed most of the assignment satisfactorily. |
| **B+** | | Good – the student has demonstrated a good understanding of much of the material, and has completed most of the assignment satisfactorily. |
| **B** | | Adequate – the student has demonstrated an understanding of the material and an ability to apply their understanding that together are sufficient to pass |
| **B-** | | Borderline failure – the student has failed to reach the standard required to pass in this subject, but not by much. The student should receive some credit for the assignment, and this may help them to pass overall. |
| **C+** | | Unsatisfactory – the student has completed some parts of the assignment successfully, but has fallen clearly short of the standard required to pass. |
| **C** | | Very poor – the student has failed to complete the simplest parts of the assignment successfully |
| **C-** | | Extremely poor – the student has failed to demonstrate the most basic competence in this subject. |

**16. Indicators of quality and standards**

- Examination conducted under supervision of Chemistry Department.
- 90% of small numbers admitted have gone on to further academic training and research.
- Positive external examiner's reports.