Accessibility statement

Chemical Theory & Computation - CHE00032M

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- **Department**: Chemistry
- **Module co-ordinator**: Dr. Martin Bates
- **Credit value**: 10 credits
- **Credit level**: M
- **Academic year of delivery**: 2020-21
  - See module specification for other years: 2019-20

Module will run

Occurrence	Teaching cycle
A	Spring Term 2020-21 to Summer Term 2020-21

Module aims

This module provides an introduction to three popular theoretical and computational methods for studying the structure of chemical systems. Theory is combined with 'hands on' practical experience in each case. Applications covering topics in solvation, structure of liquids, and quantum chemistry will be used to obtain information about individual molecules (molecular orbitals, molecular geometries, transition states) through to the structure of pure liquids and then onto mixed (solute-solvent) systems. Such theoretical and computational work has become an essential part of academic and industrial research, underpinning many practical studies to both explain results obtained in the lab, as well as to make predictions to be verified by further experiments.

Module learning outcomes

Students will gain an overview of:

- electronic structure calculation methods, including the Hartree Fock approach, post Hartree Fock methods, density functional theory and ab initio methods.
- statistical thermodynamics of liquids and solutions and an understanding the molecular basis of solvation.
- static and dynamic simulation techniques used to investigate the structure of liquids.

Module content

Quantum Chemical calculations (PBK, 6 lectures, 1x2hr workshop)
- Introduction to electronic structure theory
- Hartree-Fock approach
- Density Functional theory
- Applications using Gaussian

Solubility and Solvent Design (SS, 6 lectures, 1x2h workshop)
- Statistical thermodynamics of liquids and solutions
- Molecular basis of solvation
- Solubility in solvent mixtures
- Industrial applications (biological, pharmaceutical, green, materials, food)

Computer simulation of molecular systems (MAB, 6 lectures, 1x2h workshop)
- Monte Carlo simulation
- Molecular dynamics simulation
- Structure and dynamics of disordered and ordered liquids
- Chemical examples

Assessment

Task	Length	% of module mark
24 hour open exam Chemical Theory & Computation	N/A	70
Practical Assessed Workshop	N/A	30

Special assessment rules

None

Additional assessment information

Exam: (1.5 hr) 2 compulsory 20 mark questions, on material drawn from all three topics.

Assessed workshop: (1 hr) open book questions, on material drawn from all three topics.

Reassessment

Task	Length	% of module mark
24 hour open exam Chemical Theory & Computation	N/A	70
Practical Assessed Workshop	N/A	30

Module feedback

Workshops (summative): Oral feedback given during the workshops.

Workshop (assessed): general feedback via VLE. Marks via email.

Closed exam results with per-question breakdown are returned to the students via supervisors within 5 weeks (as per special approval by the University Teaching Committee). Outline answers are made available via the Chemistry web pages when the students receive their marks, so that they can assess their own detailed progress/achievement. The examiners' reports for each question are made available to the students via the Chemistry web pages.

Indicative reading

Computational Chemistry (Oxford Chemistry Primers)

This is a research-led course so up-to-date scientific publications will form some of the reading.

Coronavirus (COVID-19): changes to courses

The 2020/21 academic year will start in September. We aim to deliver as much face-to-face teaching as we can, supported by high quality online alternatives where we must.

Find details of the measures we're planning to protect our community.

Course changes for new students