1. KentVision Code and title of the module

CHEM7410 – Computational Chemistry

## Division and School/Department or partner institution which will be responsible for management of the module

Division of Natural Sciences (Chemistry and Forensic Science)

## The level of the module (Level 4, Level 5, Level 6 or Level 7)

Level 7

## The number of credits and the ECTS value which the module represents

15 Credits (7.5 ECTS)

## Which term(s) the module is to be taught in (or other teaching pattern)

Spring

## Prerequisite and co-requisite modules and/or any module restrictions

None

## The course(s) of study to which the module contributes

Compulsory for the following courses:

MChem Chemistry

Not available as an elective module

## The intended subject specific learning outcomes. On successfully completing the module students will be able to:

8.1 Provide a critical understanding of the field of computational chemistry.

8.2 Show how computational chemistry can provide unique insight to complement experimental chemistry.

8.3 Show how computational chemistry can deliver understanding in areas that are not, thus far, accessible to experiment.

8.4 Understand methods of computational chemistry in depth, spanning hierarchical length and time scales including: quantum mechanical, molecular dynamics (atomistic), mesoscale modelling and molecular graphics.

8.5 Use computational methods to calculate the structure, properties and processes of materials.

8.6 Evaluate computational chemistry critically with regards to scope and limitations.

8.7 Plan, design and formulate a simulation (or set of simulations) that realise a truly predictive capability.

## The intended generic learning outcomes. On successfully completing the module students will be able to:

9.1 Carry out effective research costing and planning (health and safety, ethics); ‘simulation vs experiment’.

9.2 Demonstrate problem-solving skills, relating to qualitative and quantitative information, extending to situations where evaluations have to be made on the basis of limited information.

9.3 Demonstrate time-management and organisational skills, as evidenced by the ability to plan and implement efficient and effective modes of working.

9.4 Demonstrate effective interpersonal skills, relating to the ability to engage with others and to engage in team working within a professional environment.

9.5 Exercise initiative and personal responsibility by making decisions in ‘unchartered’, complex and unpredictable situations.

## A synopsis of the curriculum

This module will introduce the student to the growing field of computational chemistry and its viability as a cost effective alternative to experiment that provides unique insight. It is critically important that an MChem student is trained in this area because many peer reviewer publications in physical, inorganic and organic chemistry include a computational component. The module will run primarily as a set of computational labs with lectures delivering the understanding, background and application of the methods used in the laboratory sessions including:

**Classical Mechanics:**

Atomistic Simulation, Force-fields, Energy Minimisation, Molecular Dynamics, Monte Carlo

**Quantum Mechanics:**

Density Functional Theory, Hartree-Fock theory, Wave-Function mechanics

**Simulation Codes:**

Examples may include for example: DL\_POLY, GULP (classical mechanics), Gaussian, Castep, Dmol (quantum mechanics)

The experiments will cover the use of computer modelling to explore the structure, properties, processes and applications of organic and inorganic materials. Typically, they might comprise:

* Simulating the adsorption of molecules on surfaces (catalysis).
* Calculating the density of states and phonon modes of materials (band gap).
* Calculating activation energy barriers of a chemical reaction (organic chemistry).
* Simulating diffusion processes (fuel cells, battery materials).
* Simulating (hard, soft) systems at the mesoscale, such as surfactant-polymer interactions and architectures.
* Quantitative Structure – Activity Relationship (QSAR) models; the application of descriptor calculations and statistical modelling to design new molecules.
* Machine Learning – intelligent computer-aided design of new materials.

## Reading list

## The University is committed to ensuring that core reading materials are in accessible electronic format in line with the Kent Inclusive Practices.

## The most up to date reading list for each module can be found on the university's [reading list pages](https://kent.rl.talis.com/index.html).

## Contact Hours

Private Study: 92

Contact Hours: 58

Total: 150

## Assessment methods

13.1 Main assessment methods

* Computational Assessment 1 (3,000 words) – 20%
* Computational Assessment 2 (3,000 words) – 20%
* Poster – 10%
* Examination (3 hours) – 50%

13.2 Reassessment methods

* Like-for-like

## Map of module learning outcomes (sections 8 & 9) to learning and teaching methods (section 12) and methods of assessment (section 13)

**Module learning outcomes against learning and teaching methods:**

| **Module learning outcome** | 8.1 | 8.2 | 8.3 | 8.4 | 8.5 | 8.6 | 8.7 | 9.1 | 9.2 | 9.3 | 9.4 | 9.5 |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Private Study | **x** | **x** | **x** | **x** |  | **x** |  |  |  | **x** |  |  |
| Lecture | **x** | **x** | **x** | **x** |  | **x** |  | **x** |  |  |  |  |
| Laboratory | **x** | **x** | **x** | **x** | **x** | **x** | **x** |  | **x** | **x** | **x** | **x** |

**Module learning outcomes against assessment methods:**

| **Module learning outcome** | 8.1 | 8.2 | 8.3 | 8.4 | 8.5 | 8.6 | 8.7 | 9.1 | 9.2 | 9.3 | 9.4 | 9.5 |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Computational Assessments | **x** | **x** | **x** | **x** | **x** | **x** | **x** |  | **x** | **x** | **x** | **x** |
| Poster | **x** | **x** | **x** | **x** | **x** | **x** | **x** |  | **x** | **x** | **x** | **x** |
| Examination | **x** | **x** | **x** | **x** | **x** | **x** |  | **x** |  |  |  |  |

## Inclusive module design

The Division recognises and has embedded the expectations of current equality legislation, by ensuring that the module is as accessible as possible by design. Additional alternative arrangements for students with Inclusive Learning Plans (ILPs)/declared disabilities will be made on an individual basis, in consultation with the relevant policies and support services.

The inclusive practices in the guidance (see Annex B Appendix A) have been considered in order to support all students in the following areas:

a) Accessible resources and curriculum

b) Learning, teaching and assessment methods

## Campus(es) or centre(s) where module will be delivered

Canterbury

## Internationalisation

Science is an international discipline with widely applicable international resonance. This module presents subject-specific knowledge generated, developed, and refined by scientists around the world. Mastery of the learning outcomes will equip students to apply the knowledge in a wide range of international contexts and these will be addressed in making the content relevant to current global issues. The Division of Natural Sciences is an international community of students and staff and group activities and teaching will provide a platform for internationally-focussed discussion.

**DIVISIONAL USE ONLY**

**Module record – all revisions must be recorded in the grid and full details of the change retained in the appropriate committee records.**

| Date approved | New/Major/minor revision | Start date of delivery of (revised) version | Section revised  (if applicable) | Impacts PLOs (Q6&7 cover sheet) |
| --- | --- | --- | --- | --- |
| 9 Dec 2021 | Minor | Sept 2022 | 5-6, 12-13 | No |
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| Revised FSO Jan 2018 |