1. KentVision Code and title of the module

CHEM6730 – Physical Chemistry 3: Computational Chemistry

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

Division of Natural Sciences (Chemistry & Forensic Science)

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

Level 6

## 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:

BSc(Hons) Chemistry

BSc(Hons) Chemistry with a Professional Placement

BSc(Hons) Chemistry with a Year Abroad

BSc(Hons) Chemistry with a Foundation Year

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 Demonstrate knowledge and systematic understanding of how computational modelling and simulation can underpin chemistry and provide unique insight – especially in areas that are not, thus far, accessible to experiment.

8.2 Demonstrate knowledge and systematic understanding of methods of modelling and simulation, spanning hierarchical length and time scales.

8.3 Apply modelling and simulation to calculate the structure and properties of materials.

8.4 Understand the use of modelling and simulation in problem-solving – extending to situations where evaluations must be made on the basis of limited information.

8.5 Plan modelling and simulation experiments.

8.6 Critique the accuracy and reliability of modelling and simulation experiments.

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

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

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

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

## A synopsis of the curriculum

Computational modelling and simulations are increasingly used in the natural sciences to complement experimental work and can be used to provide unique insight, especially when experiments are expensive, dangerous or prohibited. Here, we will introduce students to modelling and simulation approaches that a chemistry practitioner is likely to encounter in their career. Possible topics may include mesoscale modelling, classical mechanics, quantum mechanics and machine learning.

## 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: 110

Contact Hours: 40

Total: 150

## Assessment methods

13.1 Main assessment methods

* Assessed Worksheet 1 (4 hours) – 40%
* Assessed Worksheet 2 (4 hours) – 40%
* Assessed Worksheet 3 (4 hours) – 20%

13.2 Reassessment methods

* 100% Coursework

## 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 | 9.1 | 9.2 | 9.3 |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Private Study | **x** | **x** |  |  |  | **x** | **x** | **x** | **x** |
| Workshops | **x** | **x** | **x** | **x** | **x** | **x** | **x** | **x** | **x** |
| Lectures | **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 | 9.1 | 9.2 | 9.3 |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Assessed Worksheets | **x** | **x** | **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) |
| --- | --- | --- | --- | --- |
| 22 Nov 2022 | Minor | Sept 2023 | 12-14 | No |
|  |  |  |  |  |