1. **Title of the module**

CHEM7410 (CH741) - Computational Chemistry

1. **School or partner institution which will be responsible for management of the module**

Physical Sciences

1. **The level of the module (Level 4, Level 5, Level 6 or Level 7)**

Level 7

1. **The number of credits and the ECTS value which the module represents**

15 credits (7.5 ECTS)

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

Autumn and Spring

1. **Prerequisite and co-requisite modules**

Prerequisite:

Successful completion of Stage 3 of the Chemistry Programme to threshold required for progression into Stage 4

1. **The programmes of study to which the module contributes**

MChem

1. **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.

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

Have a knowledge and understanding of:

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

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

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

9.5 The ability to exercise initiative and personal responsibility. The ability to make decisions in ‘unchartered’, complex and unpredictable situations. Independent learning ability required for continuing professional development.

1. **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.

The final experiment (mini project) will be one of the students own choosing where they will plan, design and formulate a computational experiment using any computational method available and then appraise the reliability and intellectual or commercial value of the experiment.

1. **Reading list (Indicative list, current at time of publication. Reading lists will be published annually)**

* P.W Atkins, Physical Chemistry, Oxford University Press, 1998, ISBN 0198501013
* R. Chang, Physical Chemistry for the Chemical and Biological Sciences, Sausalito, California: University Science Books, 2000, ISBN 9781891389061
* Handbook of Computational Chemistry Springer eBooks, Heidelberg, Germany: Springer-Verlag Berlin Heidelberg, 2012, ISBN: 978-94-007-0710-8 (Print) 978-94-007-0711-5 (Online)
* Relevant reviewed scientific journals

1. **Learning and teaching methods**

Total contact hours: 72

Private study hours: 78

Total study hours: 150

1. **Assessment methods**
   1. Main assessment methods

Practical 1 (20%) Report containing around 3,000 words

Practical 2 (20%) Report containing around 3,000 words

Assignment (10%) Poster

Examination (50%) 3hrs written exam

13.2 Reassessment methods

Like-for-like

1. **Map of module learning outcomes (sections 8 & 9) to learning and teaching methods (section12) and methods of assessment (section 13)**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **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* |
| **Learning/ teaching method** |  |  |  |  |  |  |  |  |  |  |  |  |
| Computational Chemistry Laboratory | **X** | **X** | **X** | **X** | **X** | **X** | **X** |  | **X** | **X** | **X** | **X** |
| Lectures | **X** | **X** | **X** | **X** |  | **X** |  | **X** |  |  |  |  |
| Private study | **X** | **X** | **X** | **X** |  | **X** |  |  |  | **X** |  |  |
| **Assessment method** |  |  |  |  |  |  |  |  |  |  |  |  |
| Written examination | **X** | **X** | **X** | **X** | **X** | **X** |  | **X** |  |  |  |  |
| *Laboratory report and poster* | **X** | **X** | **X** | **X** | **X** | **X** | **X** |  | **X** | **X** | **X** | **X** |

1. **Inclusive module design**

The School 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

1. **Campus(es) or centre(s) where module will be delivered**

Canterbury

1. **Internationalisation**

Students are expected to access and compare international research outcomes when presenting their practical reports and in their assignments, as well as reflect on applications of computational chemistry with a global economic aspect.

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

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Date approved | Major/minor revision | Start date of the delivery of revised version | Section revised | Impacts PLOs (Q6&7 cover sheet) |
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Revised FSO Jan 2018