1. **Title of the module**

CH741 Computational Chemistry

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

SPS

1. **The level of the module (e.g. 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 (7.5 ECTS)

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

Term 1 and Term 2

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

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.**The learning outcomes will be met upon successful completion of the module.
   1. To provide a critical understanding of the field of computational chemistry.
   2. To show how computational chemistry can provide unique insight to complement experimental chemistry.
   3. To show how computational chemistry can deliver understanding in areas that are not, thus far, accessible to experiment.
   4. To understand methods of computational chemistry in depth, spanning hierarchical length and time scales including: quantum mechanical, molecular dynamics (atomistic), mesoscale modelling and molecular graphics.
   5. To use computational methods to calculate the structure, properties and processes of materials.
   6. To evaluate computational chemistry critically with regards to scope and limitations.
   7. To plan, design and formulate a simulation (or set of simulations) that realise a truly predictive capability.
2. **The intended generic learning outcomes.**The learning outcomes will be met upon successful completion of the module.
   1. Effective research costing and planning (health and safety, ethics); ‘simulation vs experiment’.
   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.
   3. Time-management and organisational skills, as evidenced by the ability to plan and implement efficient and effective modes of working.
   4. Interpersonal skills, relating to the ability to engage with others and to engage in team working within a professional environment.
   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.
3. **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)**

(i) P.W Atkins, Physical Chemistry, Oxford University Press, 1998, ISBN 0198501013

(ii) R. Chang , Physical Chemistry for the Chemical and Biological Sciences, Sausalito, California : University Science Books, 2000, ISBN 9781891389061

(iii) 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)

(iv) Relevant reviewed scientific journals.

1. **Learning and Teaching methods  
   Computation chemistry experiments**. The students will work through a series of prescribed computational chemistry experiments and then choose an area where they will design new experiments, which will manifest as a mini project.

**Lectures** will cover all the main branches of computational chemistry as alluded to in the synopsis

**Private study** engaging with lecture material, designing their own mini-project, further reading.

1. **Assessment methods.**This module will be assessed by examination (50%) and coursework (50%).

**A written examination** will be used to assess knowledge, understanding and application of the various flavours of computational chemistry spanning mesoscale modelling, atomistic and quantum chemistry including how computational chemistry complements experimental chemistry.

**Laboratory report and poster** The computational chemistry experiments will be written up as a formal lab report and the mini project as a poster (electronic format).

1. **Map of Module Learning Outcomes (sections 8 & 9) to Learning and Teaching Methods (section12) and methods of Assessment (section 13)**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | Subject Specific Skills | | | | | | |  | Generic Skills | | | | |
| **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** | **Hours allocated** |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Computational Chemistry Laboratory | **48** | **x** | **x** | **x** | **x** | **x** | **x** | **x** |  |  | **x** | **x** | **x** | **x** |
| Lectures | 24 | **x** | **x** | **x** | **x** |  | **x** |  |  | **x** |  |  |  |  |
| Private study | 78 | **x** | **x** | **x** | **x** |  | **x** |  |  |  |  | **x** |  |  |
| **Assessment** | **Weighting** |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Written examination | 50% | **x** | **x** | **x** | **x** | **x** | **x** |  |  | **x** |  |  |  |  |
| Laboratory report and poster | 50% | **x** | **x** | **x** | **x** | **x** | **x** | **x** |  |  | **x** | **x** | **x** | **x** |

1. **The School recognises and has embedded the expectations of current disability equality legislation, and supports students with a declared disability or special educational need in its teaching. Within this module we will make reasonable adjustments wherever necessary, including additional or substitute materials, teaching modes or assessment methods for students who have declared and discussed their learning support needs. Arrangements for students with declared disabilities will be made on an individual basis, in consultation with the University’s disability/dyslexia student support service, and specialist support will be provided where needed.**
2. **Campus(es) or Centre(s) where module will be delivered:**

Canterbury

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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.**

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| --- | --- | --- | --- | --- |
| 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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