1. **Title of the module**

LABS609 Computational Chemistry

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

Centre for Higher and Degree Apprenticeships (CHDA)

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

Level 6

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)**

Flexible delivery model

Autumn and/or Spring and/or Summer

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

N/A

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

BSc (Hons) Applied Chemical Sciences

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:**

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

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

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

9.5 Demonstrate the ability to exercise initiative and personal responsibility; the ability to make decisions in ‘unchartered’, complex and unpredictable situations; the 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 important that a chemical sciences graduate 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 written materials and recorded lectures provided online for delivery of the understanding, background and application of the methods used in the laboratory sessions, which will include:

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, (1998) Physical Chemistry, Oxford University Press.

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

Handbook of Computational Chemistry Springer eBooks, Heidelberg, Germany: Springer-Verlag Berlin Heidelberg, 2012.

Relevant reviewed scientific journals.

1. **Learning and teaching methods**

Blended Distance learning:

Contact Hours: 96

Private Study Hours: 54

Total Study Hours: 150

* 1. **Assessment methods**

Laboratory Report – weighted 25%

Poster – weighted 25%

2 hour examination – weighted 50%

The weighted average for both the overall coursework and the overall exam component must be of a pass standard.

* 1. **Reassessment Methods**

Like for like

***14.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** |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Computational Chemistry Laboratory | **x** | **x** | **x** | **x** | **x** | **x** | **x** |  |  | **x** | **x** | **x** | **x** |
| Online material/ Recorded Lectures | **x** | **x** | **x** | **x** |  | **x** |  |  | **x** |  |  |  |  |
| Private study | **x** | **x** | **x** | **x** |  | **x** |  |  |  |  | **x** |  |  |
| **Assessment**  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 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(s) recognise and have 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 – the online nature of the course, together with the use of recorded lectures, will assure that the resources for this module are accessible to all students.

b) Learning, teaching and assessment methods – again, the flexible online delivery of the module, together with the variety of assessment, ensure the inclusivity of the module.

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

Blended distance learning – delivered from Medway and Canterbury campus

1. **Internationalisation**

International vocation is an important part of Applied Chemical Science. With regards to the intended learning outcomes, in particular 8.1, the target learning outcomes within this module are applicable worldwide as part of the universal principles and techniques used in the Pharmaceutics R&D Industry. With regard to subject content, the material within the syllabus is applied to a range of international contexts.

**FACULTIES SUPPORT OFFICE USE ONLY**

**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) |
| 05/10/20 | Minor | Sep 20 | 13 | No |
|  |  |  |  |  |