Module Specification

Module Title	Computational Chemistry	Module Code	CHE305U

Credit Value	15	Level	6	Mode of Delivery	On Campus		Semester B

Pre-requisite modules	Co-requisite modules	Overlapping modules
CHE202 Structure and Reactivity of Organic Chemistry		

1) Content Description

Provide a description of the module, as it will appear in the Module Directory and on the Student Information System (approx. 70-80 words).

This module discusses key approaches in modern theoretical and computational chemistry, including HF, post-HF and DFT methods, and considers the application of such methods to study of the structure, properties and chemical reactivity of individual molecules, and further extended to the study of condensed matter.

2) Module Aims

Specify the aims of the module, i.e. the broad educational purposes for offering this module.

This module aims to provide students with an understanding of how the theories of quantum mechanics and a variety of computational approaches can be applied to the study of the structure, properties and chemical reactivity of individual molecules, and further extended to the study of condensed matter. Such knowledge and understanding will underpin studies of molecular structure and reactivity in other advanced chemistry modules.

3) Learning Outcomes

Identify the learning outcomes for this module, i.e. knowledge, skills and attributes to be developed through completion of this module. Outcomes should be referenced to the relevant QAA benchmark statements and the Framework for Higher Education Qualifications in England, Wales and Northern Ireland (2008). The SEEC Credit Level Descriptors for Further and Higher Education 2003 and Queen Mary Statement of Graduate Attributes should also be used as a guiding framework for curriculum design.

Academic Content:	
A 1	Computational methods in chemistry, including: • Force-fieldmethods; Hartree–Fock (HF), post-HF and DFT methods • Geometry-optimisation • Electronic structure; analytical frequencies • Prediction of spectra (e.g. IR, NMR, EPR)
A 2	Potential energy hypersurfaces (PEHS), and the relationship of PEHS topology to chemical structure, reactivity as well as material properties and phase-changes in matter.
A 3	Electronic structure and bonding, basic concepts of Bader's Atoms In Molecules wavefunction analyses
A 4	Introductory aspects of dynamics in chemical systems and soft condensed matter.

Disciplinary skills - able to:	
B1	Carry-out chemical calculations of intermediate complexity using commercial software (e.g. Gaussian)

B2	Interpret output data from computational chemistry calculations, and make reasonable deductions based upon such data
B3	Select appropriate models for investigation of molecular structure, properties and reactivity
B4	Relate PEHS topology to chemical structure, reactivity, material properties and phase-changes

Attributes:	
C1	Acquire and apply knowledge relating to the principles and practices of organic chemistry
C2	Produce analyses which are grounded in experimental evidence (e.g. spectroscopic data)
C3	Apply existing knowledge and skills to investigate unfamiliar problems.

4) Reading List

Provide an indicative reading list for the module. This should include key texts and/or journals but should not be an exhaustive list of materials.

Errol G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics (2nd Edition), Springer, Netherlands, 2011.
James B. Foresman and AEleen Frisch, Exploring Chemistry With Electronic Structure Methods, Gaussian, Inc, 1996.

Richard F. W. Bader, Atoms In Molecules - A Quantum Theory, Oxford University Press, Inc., 1994.

5) Teaching and Learning Profile

Provide details of the method of delivery (lectures, seminars, fieldwork, practical classes, etc.) used to enable the achievement of learning outcomes and an indicative number of hours for each activity to give an overall picture of the workload a student taking the module would be expected to undertake. This information will form the Key Information Set for each undergraduate programme and will be used to populate the KIS widget found on the QMUL programme information pages. More information can be found online about KIS. You may also wish to refer to the QAA guidance on contact hours when completing this section.

Activity Type	KIS Category	Time Spent (in hours)
Lecture	Scheduled	22
Practical Classes and Workshops	Scheduled	30
Guided Independent Study	Independent	98
	Total	150

Specify the total module notional study hours. This should be a total of the hours given for each activity. The notional study hours for each academic credit point is 10. A 15 credit point module therefore represents 150 notional study hours.

Activity Type	Total Time Spent (in hours)	Percentage of Time Spent
Scheduled learning and teaching	52	35
Placement	0	0
Independent Study	98	65
Total	150	100

Use the information provided in the box above to specify the total time spent and the percentage time spent in each category of teaching and learning activity.

6) Assessment Profile

Provide details of the assessment methods used to assess the achievement of learning outcomes.

Description	Assessment	KIS Category	Duration/Length	Percentage	Final element	Qualifying

of Assessment	Type			Weighting	of assessment	Mark
Coursework	Written Assignment, inc Essay	Coursework		50%	No	
Examination	Written Exam	Written	2.5 Hours	50%	Yes	

Final element of assessment: The assessment that takes place last. There should normally be only one element of assessment marked as final unless two assessment or submission dates occur on the same day.
Qualifying mark: A specified minimum mark that must be obtained in one or more elements of assessment in order to pass a module. This is in addition to, and distinct from, the requirement to achieve a pass in the module mark to pass the module.

Reassessment

Provide details of the reassessment methods used, specifying whether reassessment is either standard reassessment or synoptic reassessment.

○ Standard Reassessment ◉ Synoptic Reassessment

Synoptic reassessment details (if you have indicated synoptic reassessment above, please give details)		
Brief Description of Assessment	Assessment Type	Duration/Length of Examination/ Coursework
Resit Examination	Written Exam	