香港城市大學
City University of Hong Kong

SYL

Course Syllabus

offered by Department of Chemistry
with effect from Semester B 2017/18

This form is for the completion by the *Course Leader*. The information provided on this form is the official record of the course. It will be used for the City University's database, various City University publications (including websites) and documentation for students and others as required.

Please refer to the Explanatory Notes on the various items of information required.

Prepared / Last Updated by:

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Part I Course Overview

Course Title:	Computational Chemistry
Course Code:	BCH3053
Course Duration:	1 semester
Credit Units:	3 credits
Level:	B3
Proposed Area: *(for GE courses only)*	☐ Arts and Humanities ☐ Study of Societies, Social and Business Organisations ☐ Science and Technology
Medium of Instruction:	English
Medium of Assessment:	English
Prerequisites: *(Course Code and Title)*	Nil
Precursors: *(Course Code and Title)*	Nil
Equivalent Courses: *(Course Code and Title)*	Nil
Exclusive Courses: *(Course Code and Title)*	Nil

Part II Course Details

1. Abstract

(A 150-word description about the course)

This course aims to present the basic principles of computational chemistry, discussing their related applications to various areas in chemistry.

2. Course Intended Learning Outcomes (CILOs)

(CILOs state what the student is expected to be able to do at the end of the course according to a given standard of performance.)

No.	CILOs[#]	Weighting* (if applicable)	Discovery-enriched curriculum related learning outcomes (please tick where appropriate)		
			A1	*A2*	*A3*
1.	Perform a complete geometry optimization for chemical compounds.			✓	
2.	Predict the vibrational, UV/VIS and NMR spectra for chemical compounds.			✓	
3.	Locate the transition state structure(s) in simple chemical reactions.		✓	✓	
4.	Extract useful information such as electronic energy and heats of formation from the completed calculation outputs.			✓	
5.	Construct the potential energy surface connecting two (or more) stationary points.		✓	✓	
6.	Determine an appropriate method with theoretical support for a specific chemical problem.		✓		✓
** If weighting is assigned to CILOs, they should add up to 100%.*		100%			

[#] Please specify the alignment of CILOs to the Gateway Education Programme Intended Learning outcomes (PILOs) in Section A of Annex.

A1: Attitude
Develop an attitude of discovery/innovation/creativity, as demonstrated by students possessing a strong sense of curiosity, asking questions actively, challenging assumptions or engaging in inquiry together with teachers.

A2: Ability
Develop the ability/skill needed to discover/innovate/create, as demonstrated by students possessing critical thinking skills to assess ideas, acquiring research skills, synthesizing knowledge across disciplines or applying academic knowledge to self-life problems.

A3: *Accomplishments*
Demonstrate accomplishment of discovery/innovation/creativity through producing /constructing creative works/new artefacts, effective solutions to real-life problems or new processes.

3. Teaching and Learning Activities (TLAs)

(TLAs designed to facilitate students' achievement of the CILOs.)

TLA	Brief Description	CILO No.						Hours/week (if applicable)
		1	2	3	4	5	6	
Lectures	Students will learn to input molecular geometries and optimize the structures in a computer program through large group activities. (lectures)	✓						
Lectures	Students will be performing literature searches for vibrational, UV/VIS and NMR spectra of given chemical compounds and they will perform theoretical vibrational, UV/VIS and NMR spectral prediction and make critical comparisons. (lectures)		✓					
Lectures and/or tutorials	Through a number of case studies (e.g., SN2 reaction and isomerization), students have to locate the transition state structures and verify the nature of the transition states along the reaction pathway by transition vectors analysis. (lectures and/or tutorials)			✓				
Tutorials	Student-centred learning and group project will form the basis for this activity, designed to give students practice in understanding energetic and stability aspects of molecules. (tutorials)				✓			
Tutorials	Tutorial teaching methods will enable students to construct the potential energy surface and examine related properties. (tutorials)					✓		
Projects	Project based activity will be used to guide students to master the knowledge on the reliability of various theoretical theories in computational chemistry.	✓	✓	✓	✓	✓	✓	

Lectures and tutorials covering CILOs1-6 are expected to be conducted in the computer center. Every student will be using a PC and learning this course interactively.

4. Assessment Tasks/Activities (ATs)

(ATs are designed to assess how well the students achieve the CILOs.)

Assessment Tasks/Activities	CILO No.						Weighting*	Remarks
	1	2	3	4	5	6		
Continuous Assessment: 70%								
Homework	✓	✓	✓		✓	✓	22%	
Quizzes, tests and reports	✓	✓	✓		✓	✓	22%	
Individual project	✓	✓	✓	✓	✓	✓	26%	
Examination: 30% (duration: 2 hours)								
** The weightings should add up to 100%.*							100%	

Starting from Semester A, 2015-16, students must satisfy the following minimum passing requirement for BCH courses:

"A minimum of 40% in both coursework and examination components."

5. Assessment Rubrics

(Grading of student achievements is based on student performance in assessment tasks/activities with the following rubrics.)

Assessment Task	Criterion	Excellent (A+, A, A-)	Good (B+, B, B-)	Fair (C+, C, C-)	Marginal (D)	Failure (F)
1. Homework	Ability to understand and finish the homework.	Student is expected to show strong evidence of subject matter and great familiarity with knowledge.	Student is expected to demonstrate evidence of subject, evidence of familiarity with knowledge.	Student is expected to show sufficient evidence of the subject and little familiarity with knowledge.	Student is expected to demonstrate little familiarity with the subject matter and limited evidence of knowledge.	Student shows no evidence of familiarity with the subject matter and irrelevant understanding of knowledge.
2. Quizzes, tests and reports	Ability to comprehend and complete the tests and reports.	Student is expected to show strong evidence of subject matter and great familiarity with knowledge.	Student is expected to demonstrate evidence of subject, evidence of familiarity with knowledge.	Student is expected to show sufficient evidence of the subject and little familiarity with knowledge.	Student is expected to demonstrate little familiarity with the subject matter and limited evidence of knowledge.	Student shows no evidence of familiarity with the subject matter and irrelevant understanding of knowledge.
3. Individual project	Capacity to understand the scope of project and complete the tasks.	Student is expected to show strong evidence of subject matter and great familiarity with knowledge.	Student is expected to demonstrate evidence of subject, evidence of familiarity with knowledge.	Student is expected to show sufficient evidence of the subject and little familiarity with knowledge.	Student is expected to demonstrate little familiarity with the subject matter and limited evidence of knowledge.	Student shows no evidence of familiarity with the subject matter and irrelevant understanding of knowledge.
4. Examination	Ability to comprehend and finish the examination paper.	Student is expected to show strong evidence of original thinking; good organization, capacity to analyse and synthesize the subject matter; superior grasp of knowledge is required.	Student is expected to demonstrate evidence of grasp of subject, some evidence of critical capacity and analytic ability; reasonable understanding of issues; evidence of familiarity with knowledge.	Student is expected to show sufficient evidence of the subject, little evidence of critical capacity and analytic ability; fair understanding of issues.	Student is expected to demonstrate little familiarity with the subject matter to enable the student to progress without repeating the course.	Student shows no evidence of familiarity with the subject matter; weakness in critical and analytic skills; limited, or irrelevant understanding of knowledge.

Part III Other Information (more details can be provided separately in the teaching plan)

1. Keyword Syllabus

(An indication of the key topics of the course.)

Electronic Structure Methods

Hartree-Fock Theory. Electron Correlation. Perturbation Theory. Density Functional Theory. Basis Set Approximation.

Atomic and Molecular Properties

Atomic Charge and Electron Density. Symmetry and Point group. Electronic State. Wavefunction. Chemical Bonding and Molecular Orbitals.

Using Quantum Chemistry Programs

Gaussian-03 Program Interface. Input of Moleculer Structure. Z-matrix Construction. Viewing the Molecules Using GaussView.

Structure

Geometry Optimizations. Minimum and Stable Structure. Saddle Point and Transition Structure. Predictions of Vibrational Frequencies and Spectra. Predictions of Chemical Shifts and NMR Spectra.

Energetic

Electronic Energy. Zero-Point Vibrational Energy. Transition Barrier and Activation Energy. Conformational Energetics. Reaction Energetics. Enthalpy of Formation. Bond Dissociation Energy. Ionization Energy. Isomerization Energy and Barrier.

Reactivity

Potential Energy Surface. Reaction Mechanism.

Spectral Simulation

IR, UV/VIS and NMR spectra

2. Reading List

2.1 Compulsory Readings

(Compulsory readings can include books, book chapters, or journal/magazine articles. There are also collections of e-books, e-journals available from the CityU Library.)

1.	Quantum Chemistry and Spectroscopy, Thomas Engel, Pearson, 2nd Ed., 2010.
2.	Introduction to Computation Chemistry, Frank Jensen, Wiley, 2nd Ed., 2006.
3.	Exploring Chemistry with Electronic Structure Methods, James B. Foresman and Æleen Frisch, Gaussian; 2nd Ed., 1996.
…	

2.2 Additional Readings

(Additional references for students to learn to expand their knowledge about the subject.)

Nil

Annex
(for GE courses only)

A. Please specify the Gateway Education Programme Intended Learning Outcomes (PILOs) that the course is aligned to and relate them to the CILOs stated in Part II, Section 2 of this form:

GE PILO	**Please indicate which CILO(s) is/are related to this PILO, if any** ***(can be more than one CILOs in each PILO)***
PILO 1: Demonstrate the capacity for self-directed learning	
PILO 2: Explain the basic methodologies and techniques of inquiry of the arts and humanities, social sciences, business, and science and technology	
PILO 3: Demonstrate critical thinking skills	
PILO 4: Interpret information and numerical data	
PILO 5: Produce structured, well-organised and fluent text	
PILO 6: Demonstrate effective oral communication skills	
PILO 7: Demonstrate an ability to work effectively in a team	
PILO 8: Recognise important characteristics of their own culture(s) and at least one other culture, and their impact on global issues	
PILO 9: Value ethical and socially responsible actions	
PILO 10: Demonstrate the attitude and/or ability to accomplish discovery and/or innovation	

GE course leaders should cover the mandatory PILOs for the GE area (Area 1: Arts and Humanities; Area 2: Study of Societies, Social and Business Organisations; Area 3: Science and Technology) for which they have classified their course; for quality assurance purposes, they are advised to carefully consider if it is beneficial to claim any coverage of additional PILOs. General advice would be to restrict PILOs to only the essential ones. (Please refer to the curricular mapping of GE programme: http://www.cityu.edu.hk/edge/ge/faculty/curricular_mapping.htm.)

B. Please select an assessment task for collecting evidence of student achievement for quality assurance purposes. Please retain at least one sample of student achievement across a period of three years.

Selected Assessment Task