CHEM3053: COMPUTATIONAL CHEMISTRY

Effective Term
Semester A 2025/26

Part I Course Overview

Course Title
Computational Chemistry

Subject Code
CHEM - Chemistry
Course Number
3053

Academic Unit
Chemistry (CHEM)

College/School
College of Science (SI)

Course Duration
One Semester

Credit Units
3

Level
B1, B2, B3, B4 - Bachelor's Degree

Medium of Instruction
English

Medium of Assessment
English

Prerequisites
Nil

Precursors
Nil

Equivalent Courses
BCH3053 Computational Chemistry

Exclusive Courses
Nil

Part II Course Details

Abstract
The aim of the course is to introduce students to the basic principles of computational chemistry and provide them with the skills to apply computational methods to tackle problems and explain phenomena in chemistry. Through the course,

students will gain an understanding of the fundamentals of computational chemistry, including the underlying theories and algorithms. They will learn how to utilize computational tools and software to model chemical systems, simulate reactions, and analyze the results. The goal is to equip students with the knowledge and practical expertise to leverage computational chemistry techniques to address a variety of research and applied problems in the field of chemistry.

Course Intended Learning Outcomes (CILOs)

	CILOs	Weighting (if app.)	DEC-A1	DEC-A2	DEC-A3
1	Perform a complete geometry optimization for chemical compounds and locate the transition state structure(s) in simple chemical reactions.	20	x	x	
2	Predict the vibrational, UV/VIS and NMR spectra for chemical compounds.	20		x	
3	Extract useful information such as electronic energy and heats of formation from the completed calculation outputs.	20		x	
4	Construct the potential energy surface connecting two (or more) stationary points.	17	x	x	
5	Determine an appropriate method with theoretical support for a specific chemical problem.	23	x		x

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 real-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.

Learning and Teaching Activities (LTAs)

	LTAs	Brief Description	CILO No.	Hours/week (if applicable)
1	Lectures and/or tutorials	Students will learn to construct the molecular structures and optimize the structures in a computer program through large group activities. Through a number of case studies (e.g., SN2 reaction and isomerization), students will be guided to locate the transition state structures and verify the nature of the transition states along the reaction pathway by transition vectors analysis.	1	
2	Lectures and/or tutorials	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.	2	
3	Lectures and/or tutorials	Students will learn to model the molecules in a computer and understand the stability based on the energetics and heat of formations calculations.	3	
4	Lectures and/or tutorials	Lectures and tutorials will enable students to construct the potential energy surface, identify the minimum and maximum stationary points and examine their properties on the surface.	4	
5	Project and presentation	Project based activity will be used to guide students to master the knowledge on the applications of various theoretical theories and computational techniques in chemistry.	1, 2, 3, 4, 5	

Additional Information for LTAs

Lectures and tutorials covering CILOs1-5 are expected to be conducted in the computer center. Every student will be using a PC and learning this course interactively.

Assessment Tasks / Activities (ATs)

	ATs	CILO No.	Weighting (%)	Remarks ("-" for nil entry)	Allow Use of GenAI?
1	Homework	1, 2, 3, 4	12	-	Yes
2	Quizzes, and tests	1, 2, 3, 4	15	-	Yes
3	Individual project and presentation	1, 2, 3, 4, 5	23	-	Yes

Continuous Assessment (%)

50

Examination (%)

50

Examination Duration (Hours)

2

Minimum Continuous Assessment Passing Requirement (%)

40

Minimum Examination Passing Requirement (%)

40

Assessment Rubrics (AR)

Assessment Task

Homework

Criterion

Ability to understand and finish the homework.

Excellent (A+, A, A-)

Student is expected to show strong evidence of subject matter and great familiarity with knowledge.

Good (B+, B, B-)

Student is expected to demonstrate evidence of subject, evidence of familiarity with knowledge.

Fair (C+, C, C-)

Student is expected to show sufficient evidence of the subject and little familiarity with knowledge.

Marginal (D)

Student is expected to demonstrate little familiarity with the subject matter and limited evidence of knowledge.

Failure (F)

Student shows no evidence of familiarity with the subject matter and irrelevant understanding of knowledge.

Assessment Task

Quizzes, tests and reports

Criterion

Ability to comprehend and complete the tests and reports.

Excellent (A+, A, A-)
Student is expected to show strong evidence of subject matter and great familiarity with knowledge.

Good (B+, B, B-)
Student is expected to demonstrate evidence of subject, evidence of familiarity with knowledge.

Fair (C+, C, C-)
Student is expected to show sufficient evidence of the subject and little familiarity with knowledge.

Marginal (D)
Student is expected to demonstrate little familiarity with the subject matter and limited evidence of knowledge.

Failure (F)
Student shows no evidence of familiarity with the subject matter and irrelevant understanding of knowledge.

Assessment Task
Individual project

Criterion
Capacity to understand the scope of project and complete the tasks.

Excellent (A+, A, A-)
Student is expected to show strong evidence of subject matter and great familiarity with knowledge.

Good (B+, B, B-)
Student is expected to demonstrate evidence of subject, evidence of familiarity with knowledge.

Fair (C+, C, C-)
Student is expected to show sufficient evidence of the subject and little familiarity with knowledge.

Marginal (D)
Student is expected to demonstrate little familiarity with the subject matter and limited evidence of knowledge.

Failure (F)
Student shows no evidence of familiarity with the subject matter and irrelevant understanding of knowledge.

Assessment Task
Examination

Criterion
Ability to comprehend and finish the examination paper.

Excellent (A+, A, A-)
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.

Good (B+, B, B-)
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.

Fair (C+, C, C-)

Student is expected to show sufficient evidence of the subject, little evidence of critical capacity and analytic ability; fair understanding of issues.

Marginal (D)

Student is expected to demonstrate little familiarity with the subject matter to enable the student to progress without repeating the course.

Failure (F)

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

Keyword Syllabus

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-16 Program Interface. Input of Molecular Structure. 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

Reading List

Compulsory Readings

	Title
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.

Additional Readings

	Title
1	Nil