هيئة تقويم التعليم والتدريب
Education & Training Evaluation Commission

Course Specifications

Course Title:	**Computational Chemistry**
Course Code:	**2044212-2**
Program:	**Bachelor in Chemistry**
Department:	**Department of Chemistry**
College:	**College of Sciences**
Institution:	**Taif University**

Table of Contents

A. Course Identification

1. Credit hours:	**2 (1 Theoretical, 1 Lab)**
2. Course type	
a.	University ☐ College ☐ Department ☑ Others ☐
b.	Required ☐ Elective ☑
3. Level/year at which this course is offered:	**8th Level / 4th Year**
4. Pre-requisites for this course (if any)**:**	**NA**
5. Co-requisites for this course (if any)**:**	**NA**

6. Mode of Instruction (mark all that apply)

No	Mode of Instruction	Contact Hours	Percentage
1	**Traditional classroom**	1 Theoretical and 3 Practical hours/ Week	100%
2	**Blended**	--	--
3	**E-learning**	--	--
4	**Distance learning**	--	--
5	**Other (Laboratory)**	--	--

7. Contact Hours (based on academic semester)

No	Activity	Contact Hours
1	**Lecture**	15
2	**Laboratory/Studio**	45
3	**Tutorial**	--
4	**Others** (specify)	--
	Total	**60**

B. Course Objectives and Learning Outcomes

1. Course Description

This introductory course in computational chemistry discusses the fundamentals of building the theoretical models for calculating the optimum molecular geometry and the lowest molecular energy.

2. Course Main Objective

Use computational tools to increase the understanding of materials, theoretical topics and computational techniques in chemistry and to provide a foundation in the concepts of the theoretical chemistry.

3. Course Learning Outcomes

	CLOs	Aligned PLOs
1	**Knowledge and Understanding:**	
1.1	Define computational chemistry and its discipline	K1
1.2	Recognize different electronic structure methods in computational chemistry	K2
2	**Skills:**	
2.1	Distinguish between electronic structure methods and ab initio methods	S1

CLOs		Aligned PLOs
2.2	Design molecular mechanics and molecular dynamics chemical experiments	S2
3	**Values:**	
3.1	Participate in the development of the performance of work teams	V1

C. Course Content

No	List of Topics	Contact Hours
1	Scope of computational chemistry; course topics; review of key concepts.	1
2	Introduction of computational chemistry.	1
3	Cartesian coordinates and Z-matrix - Geometry optimization.	2
4	The Born-Oppenheimer approximation, potential energy surfaces, local and global minima, maxima, transition states.	2
5	Single point Energy Calculations.	1
6	Molecular Mechanics /Force Field Methods: Introduction to molecular mechanics; Bond stretching term, Bond angle term, Dihedral angle term.	2
7	Molecular Dynamics simulation.	2
8	Molecular Dynamics algorithm - Mont Carlo Simulation.	2
9	Limitations of the MD technique.	1
10	The Hartree Fock Approximation-Schroëdinger's Equation.	1
Total		**15**

Lab Content

No	List of Topics	Contact Hours
1	Introduction to computational chemistry.	3
2	Overview on ChemBio 3D Ultra Software.	3
3	Building and displaying molecules on ChemBio 3D Ultra Software.	6
4	Method of calculating bond distance using ChemBio 3D Ultra Software.	6
5	Method of calculating bond angle using ChemBio 3D Ultra Software.	6
6	Method of calculating torsion angle using ChemBio 3D Ultra Software**.**	6
7	Calculating and displaying Z-matrix (internal coordinate) using ChemBio 3D Ultra Software.	3
8	Calculating and displaying Cartesian coordinate table using ChemBio 3D Ultra Software.	3
9	Calculating atomic charges of a molecule using ChemBio 3D Ultra Software.	6
10	Computing properties of a molecules using ChemBio 3D Ultra Software.	3
Total		**45**

D. Teaching and Assessment

1. Alignment of Course Learning Outcomes with Teaching Strategies and Assessment Methods

Code	Course Learning Outcomes	Teaching Strategies	Assessment Methods
1.0	**Knowledge and Understanding**		
1.1	Define computational chemistry and its discipline.	Lecture and small group discussion	Written Exam

Code	Course Learning Outcomes	Teaching Strategies	Assessment Methods
1.2	Recognize different electronic structure methods in computational chemistry.	Lecture and small group demonstrations	Written Exam
2.0	**Skills**		
2.1	Distinguish between electronic structure methods and ab initio methods.	Discussion	Homework Assignments
2.2	Design molecular mechanics and molecular dynamics chemical experiments.	Problem-Solving	Practical tasks and Exam
3.0	**Values**		
3.1	Participate in the development of the performance of work teams.	Collaborative Learning	Individual presentations

2. Assessment Tasks for Students

#	Assessment task*	Week Due	Percentage of Total Assessment Score
1	Homework Assignments	Throughout Semester	5%
2	Individual presentations	Throughout Semester	5%
3	Periodical Exam	7/8	20%
4	Mid Term Exam	11/12	10%
5	Practical tasks	Throughout Semester	15%
6	Final practical Exam	15	5%
7	Final exam	16	40%

***Assessment task** (i.e., written test, oral test, oral presentation, group project, essay, etc.)

E. Student Academic Counseling and Support

Arrangements for availability of faculty and teaching staff for individual student consultations and academic advice :

Commitment to the rules of the Academic Advising Department at the university in accordance with the academic guidance manual approved by the university and the attached forms, there are different arrangements made by teaching staff to support student consultations including;
- Office hours: 8 hours per a week for each academic member.
- Academic guidance: an academic member has a number of students to guide them throughout degree journey.

F. Learning Resources and Facilities

1. Learning Resources

Required Textbooks	• Essentials of Computational Chemistry, Christopher J. Cramer (2004). John Wiley & Sons (USA), Latest Edition. ISBN: 978-0-470-09182-1. • Introduction to Computational Chemistry, Frank Jensen (2017). John Wiley & Sons (USA), Latest Edition. ISBN: 978-1-118-82599-0.
Essential References Materials	• Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems, David Young (2001). John Wiley & Sons, Inc. (USA), Latest Edition. ISBN: 9780471333685.

	• Encyclopedia of Computational Chemistry, Paul von Ragué Schleyer (1998). Wiley (USA), Latest Edition. ISBN 0-471-96588-6.
Electronic Materials	• Saudi Digital Library (SDL)
Other Learning Materials	• Learning Management System (Blackboard) • Computer programs: Chem Bio 3D Ultra, Gaussian Software

2. Facilities Required

Item	Resources
Accommodation (Classrooms, laboratories, demonstration rooms/labs, etc.)	A classroom with movable tables and chairs conducive to group discussion and teamwork
Technology Resources (AV, data show, Smart Board, software, etc.)	• Computer and data show with Wi-Fi access. • Computer programs: Chem Bio 3D Ultra, Gaussian Software
Other Resources (Specify, e.g. if specific laboratory equipment is required, list requirements or attach a list)	--

G. Course Quality Evaluation

Evaluation Areas/Issues	Evaluators	Evaluation Methods
Effectiveness of Teaching and assessment	Students	Survey (indirect method)
Extent of achievement of course learning outcomes	Program leader	Reports (Direct method)
Quality of learning resources	Peer referees Students	Reports (Direct method) Survey (indirect method)

Evaluation areas (e.g., Effectiveness of teaching and assessment, Extent of achievement of course learning outcomes, Quality of learning resources, etc.)
Evaluators (Students, Faculty, Program Leaders, Peer Reviewer, Others (specify)
Assessment Methods (Direct, Indirect)

H. Specification Approval Data

Council / Committee	**Department Council/ Quality assurance committee**
Reference No.	7-3-1445
Date	27/2/1445 HJ 12/09/2023 G