Course Specification
(Bachelor)

Course Title:	Computational Chemistry
Course Code:	CEM 380
Program:	Industrial Chemistry
Department:	CHEMISTRY
College:	COLLEGE OF SCIENCE
Institution:	MAJMAAH UNIVERSITY
Version:	TP-153
Last Revision Date:	10/12/2024

Table of Contents

A. General information about the course:

1. Course Identification

1. Credit hours: (3)					
2. Course type					
A.	☐University	☐College	☐Department	☐Track	☐Others
B.	☐Required		☒ Elective		
3. Level/year at which this course is offered: (8th/ 4th)					
4. Course General Description:					
The course addresses computer-based calculations within chemistry. The course integrates theory with practical computation elements applied within the fields of environmental chemistry, protein chemistry and medicinal chemistry. The course comprises both theory and practical application of important concepts within quantum chemistry and molecular mechanics. Central concepts for the computer-based application of organic molecules within quantum chemistry will be described and discussed. The focus within molecular mechanics is on describing and discussing the practical application of organic molecules, including proteins.					
5. Pre-requirements for this course (if any)**:**					
CEM344					
6. Co-requisites for this course (if any)**:**					
None					
7. Course Main Objective(s):					
• Achieve a sufficient understanding of the theory behind computational chemistry and give students a sound appreciation of the many ways in which computational chemistry can be used to solve chemical problems. • Employ several programs (such as Gaussian, MOPAC and HyberChem) to calculate the structures and properties of molecules and solids. • The students will be mentioned to prepare an essay or a report from literature using the library, database services, and/or websites to follow up and update the new topics of the subject of the course.					

2. Teaching mode (mark all that apply)

No	Mode of Instruction	Contact Hours	Percentage
1	Traditional classroom		60%
2	E-learning		10%
3	Hybrid • Traditional classroom • E-learning		30%
4	Distance learning		0

3. Contact Hours (based on the academic semester)

No	Activity	Contact Hours
1.	**Lectures**	30
2.	**Laboratory/Studio**	0
3.	**Field**	0
4.	**Tutorial**	0
5.	**Others (specify)**	15
Total		45

B. Course Learning Outcomes (CLOs), Teaching Strategies and Assessment Methods

Code	Course Learning Outcomes	Code of PLOs aligned with the program	Teaching Strategies	Assessment Methods
1.0	**Knowledge and understanding**			
1.1	**Understand theories of computational chemistry and recognize its importance in solving chemical problems.**	**K1**	**- lectures (PowerPoint) and Video related to the topic. - Discussions - E-learning - Self-learning**	**- Midterms - Quizzes - Homework - Class participation - Encourage students to search the Internet for everything related to**

Code	Course Learning Outcomes	Code of PLOs aligned with the program	Teaching Strategies	Assessment Methods
				- Homework on the blackboard - Final exam - E-exam.
2.0	**Skills**			
2.2	Communicate effectively orally and written using appropriate presentation methods for different chemical issues with recipients of different types	S2	Cooperative learning -Problem Solving - Interactive teaching - Discussion and dialogue - Active Learning - Peer Learning - Encourage students to work as team in order to raise the spirit of cooperation among students	- Assignment - Homework -Research papers Request a share Presentation and homework and then presented them on the class. -Present a presentation for each group
2.3	Demonstrate the ability to apply various chemical software to calculate structures and properties of molecules.	S3		
3.0	**Values, autonomy, and responsibility**			
3.2	Shows the ability to deal with difficult situations and work under pressure.	V2	Assignments (individual or group) at regular intervals to solve and submit on time. • Participation of students in classroom discussion and problem solving sessions • Team work reports and presentations	- Observing student's participation in group activity. - Checklist of the tasks carried out by the student. Observing student's participation in group discussion. - Checklist of student's
3.3	Take the personality and responsibility for their own learning.	V3		

Code	Course Learning Outcomes	Code of PLOs aligned with the program	Teaching Strategies	Assessment Methods
			(data collection, internet search, data processing, analysis and reporting) • Use digital libraries for literature survey. • Use E-Learning Systems for the communication with lecturer through the course work.	punctuality in submitting work on time.

C. Course Content

No	List of Topics	Contact Hours
1.	Introduction	3
2.	Molecular mechanics	6
3.	Simulations of molecular ensembles	6
4.	Foundations of molecular orbital theory	6
5.	Semiempirical implementations of molecular orbital theory	6
6.	Applications using software	6
7.	Ab Initio implementations of Hartree-Fockmolecular orbital theory	3
8.	Density functional theory	3
Total		45

D. Students Assessment Activities

No	Assessment Activities *	Assessment timing (in week no)	Percentage of Total Assessment Score
1.	Homework	End of topic	5%
2.	Quizzes	One/semester	5%
3.	Presentation	5th	10%
4.	First midterm exam	9th	15%
5.	Second midterm exam	10th	15%

No	Assessment Activities *	Assessment timing (in week no)	Percentage of Total Assessment Score
6.	E. exam	12th	10%
7.	Final written Exam	End of topic	40%

*Assessment Activities (i.e., Written test, oral test, oral presentation, group project, essay, etc.).

E. Learning Resources and Facilities

1. References and Learning Resources

Essential References	International Journal of Quantum Chemistry Journal of Molecular Modeling
Supportive References	- Essentials of Computational Chemistry: Theories and models, Christopher J Cramer, WILEY, 2004. - Introduction to Computational Chemistry, Frank Jenson, WILEY, 2007.
Electronic Materials	www.elsiver.com www.springer.com www.wiley.com
Other Learning Materials	Computational chemistry software packages will be considered whenever appropriate.

2. Required Facilities and equipment

Items	Resources
facilities (Classrooms, laboratories, exhibition rooms, simulation rooms, etc.)	Classrooms, E- learning, blackboard
Technology equipment (projector, smart board, software)	Computer Halls access for the students will be helpful in doing their tasks during the course.
Other equipment (depending on the nature of the specialty)	Computational software will be helpful such as hyperchem program package.

F. Assessment of Course Quality

Assessment Areas/Issues	Assessor	Assessment Methods
Effectiveness of teaching	students	students
Effectiveness of Students assessment	Program/Department Instructor	Program/Department Instructor
Quality of learning resources	Program/Department Instructor	Program/Department Instructor

Assessment Areas/Issues	Assessor	Assessment Methods
The extent to which CLOs have been achieved	Peer review	Peer review
Other	None	

Assessors (Students, Faculty, Program Leaders, Peer Reviewers, Others (specify)

Assessment Methods (Direct, Indirect)

G. Specification Approval

COUNCIL /COMMITTEE	**CHEMISTRY DEPARTMENT COUNCIL**
REFERENCE NO.	**7**
DATE	**14-6-1446 H**