هيئة تقويم التعليم والتدريب
Education & Training Evaluation Commission

اعتماد NCAAA T4 2020

Course Specifications

Course Title:	**Quantum Chemistry**
Course Code:	**4023553-2**
Program:	**Chemistry**
Department:	**Chemistry**
College:	**Faculty of Applied Science**
Institution:	**Umm Al-Qura University**

Table of Contents

A. Course Identification

1. Credit hours: 2
2. Course type **a.** University ☐ College ☐ Department ☑ Others ☐ **b.** Required ☑ Elective ☐
3. Level/year at which this course is offered: 3rd level/2nd year
4. Pre-requisites for this course (if any)**: General chemistry2 + calculus**
5. Co-requisites for this course (if any)**: none**

6. Mode of Instruction (mark all that apply)

No	Mode of Instruction	Contact Hours	Percentage
1	**Traditional classroom**	√	80 %
2	**Blended**		
3	**E-learning**	√	20 %
4	**Distance learning**		
5	**Other**		

7. Contact Hours (based on academic semester)

No	Activity	Contact Hours
1	**Lecture**	22
2	**Laboratory/Studio**	
3	**Tutorial**	
4	**Others** (specify)	10
	Total	32

B. Course Objectives and Learning Outcomes

1. Course Description

Quantum Chemistry course provide the students with the necessary theoretical background of the quantum theory, derivation of various equations of quantum mechanics and their applications on atoms and molecules.

2. Course Main Objective

By the end of this course student will be able to :

1. Describe the fundamental principles of quantum chemistry.
2. State the fundamental postulates of quantum mechanics.
3. Develop physical intuition, mathematical reasoning, and problem solving skills..
4. Write the solution of Schrodinger equation for some simple systems.
5. Be further prepared for the necessarily rigorous sequence in chemistry courses needed the quantum chemistry

3. Course Learning Outcomes

CLOs		Aligned PLOs
1	**Knowledge and Understanding**	
1.1	Illustrate, qualitatively and quantitatively, the role of photons in understanding phenomena like the photoelectric effect and Compton scattering.	K2
1.2	Describe the experiments displaying wave like behavior of matter, and how this motivates the need to replace classical mechanics by a wave equation of motion for matter (the Schrödinger equation).	K2
1.3	Mention the basic concepts and principles of quantum mechanics: The Schrödinger equation, the wave function and its physical interpretation, Eigen values and Eigen functions, expectation values and uncertainty.	
2	**Skills :**	
2.1	Solve the Schrödinger equation for simple one-dimensional systems and conclude the probabilities, Eigen and expectation values for these systems.	S5
2.2	Apply the particle-in-a-box model to π electrons in conjugated molecules.	S3
3	**Values:**	
3.1	Work effectively both in a team, and independently on solving chemistry problems.	C2
3.2	Use IT and web search engines for collecting information**.**	C3

C. Course Content

No	List of Topics	Contact Hours
1	Basics of Quantum Theory – Introduction to Quantum Mechanics And Its Origin – Properties of Wave Function.	2
2	Solution of Schrödinger Equation – Applications of Schrödinger Equation - A Particle Moving in A Box With Different, One – Two – Three, Dimensions - Predict the Wave Function Equation and the Energy in Each Case.	4
3	Operators and its Importance in Quantum Chemistry - Eigen Functions and Eigen Values	2
4	Schrödinger Equation Of Hydrogen Atom- Wave Function Equation and Energy	4
5	Different Quantum Numbers and their Uses in Describing the Orbitals and the Energy Levels.	2
6	Quantum Theory and Molecular Structure – Born-Oppenheimer Approximation.	2
7	Revision	2
8	Molecular Orbital Theory and Molecular Structure-Linear Combination of Atomic Orbitals (LCAO).	2
9	Application of Molecular Orbital Theory on Homonuclear Molecules.	2
10	Application of Molecular Orbital Theory on Heteronuclear Molecules	2 E. L
11	Overlap Matrix- Correlation Diagrams.	2 E. L
12	Revision	2 E. L
Total		22

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	Illustrate, qualitatively and quantitatively, the role of photons in understanding phenomena like the photoelectric effect and Compton scattering.	Lecture	quiz
1.2	Describe the experiments displaying wave like behavior of matter, and how this motivates the need to replace classical mechanics by a wave equation of motion for matter (the Schrödinger equation).	Lecture	exam
1.3	Mention the basic concepts and principles of quantum mechanics: The Schrödinger equation, the wave function and its physical interpretation, Eigen values and Eigen functions, expectation values and uncertainty.	discussion	quiz
2.0	**Skills**		
2.1	Solve the Schrödinger equation for simple one-dimensional systems and conclude the probabilities, Eigen and expectation values for these systems.	lecture	exam
2.2	Apply the particle-in-a-box model to π electrons in conjugated molecules.	lecture	quiz
3.0	**Values**		
3.1	Work effectively both in a team, and independently on solving chemistry problems.	group discussion	Observation of group's team work performance
3.2	Use IT and web search engines for collecting information.	presentation	Observation by the instructor

2. Assessment Tasks for Students

#	Assessment task*	Week Due	Percentage of Total Assessment Score
1	Assignments and activities	All weeks	10%
2	E-learning	All weeks	10%
3	Mid-term Exam	6	30%
4	Final Exam. (2 hours exam)	12	50%

***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 :

- We have faculty members to provide counseling and advice.
- Office hours: During the working hours weekly.
- Academic Advising for students

F. Learning Resources and Facilities

1.Learning Resources

Required Textbooks	1- Ajit J Thakkar, Quantum Chemistry, Morgan & Claypool Publishers, 2014. 2- Donald A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
Essential References Materials	Journal of Molecular Structure (Elsevier)
Electronic Materials	• http//:en.wikipedia.org/wiki/ • http//:www.chemweb.com/ • Websites on the internet relevant to the topics of the course
Other Learning Materials	

2. Facilities Required

Item	Resources
Accommodation (Classrooms, laboratories, demonstration rooms/labs, etc.)	• **Classrooms capacity (30) students.** • **Providing hall of teaching aids including computers and projector.**
Technology Resources (AV, data show, Smart Board, software, etc.)	▪ **Room equipped with computer and projector and TV.**
Other Resources (Specify, e.g. if specific laboratory equipment is required, list requirements or attach a list)	• **No other requirements**

G. Course Quality Evaluation

Evaluation Areas/Issues	Evaluators	Evaluation Methods
Effectiveness of teaching and assessment	Students	questionnaire (indirect)
Extent of achievement of course learning outcomes	Program Leader	results data analysis (direct) and questionnaire (indirect)
Quality of learning resources	Course instructor	questionnaire (indirect)

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	**Dr. Jabir H. Al-Fahemi**
Reference No.	
Date	10/03/2022

Head of Chemistry Department

Dr Moataz Morad