Course Specifications

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

Table of Contents

A. Course Identification

1. Credit hours:	2 h (**theoretical**)
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 chemistry1 + 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	30	100
2	Blended		
3	E-learning		
4	Correspondence		
5	Other		

7. Actual Learning Hours (based on academic semester)

No	Activity	Learning Hours
Contact Hours		
1	Lecture	30
2	Laboratory/Studio	
3	Tutorial	
4	Others (specify)	
	Total	30
Other Learning Hours*		
1	Study	30
2	Assignments	8
3	Library	3
4	Projects/Research Essays/Theses	3
5	Others(specify) Quizzes and Exam preparation	20
	Total	64

*The length of time that a learner takes to complete learning activities that lead to achievement of course learning outcomes, such as study time, homework assignments, projects, preparing presentations, library times

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 need the quantum chemistry

3. Course Learning Outcomes

	CLOs	Aligned PLOs
1	**Knowledge:**	
1.1	List the historical development of the Origins of quantum theory	K2
1.2	Illustrate, qualitatively and quantitatively, the role of photons in understanding phenomena like the photoelectric effect and Compton scattering.	K2
1.3	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
1.4.	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.	K5
1.5	Define the concepts of spin and angular momentum, as well as their quantization- and addition rules.	K2
1.6	Explain physical properties of atoms and molecules based on quantum Chemical formulations.	K6
1.7	Describe a Qualitative treatment of the LCAO-MO for homonuclear and heteronuclear diatomic molecules as a well as Simple Hückel Molecular Orbital theory.	K5
2	**Skills :**	
2.1	Give concise physical interpretations and discussions of quantum mechanics postulations in molecular orbitals treatment.	S2
2.2	Solve the Schrödinger equation for simple one-dimensional systems and conclude the probabilities, Eigen and expectation values for these systems.	S5
2.3	Apply the particle-in-a-box model to π electrons in conjugated molecules.	S3
2.4	Compare between the different energies of the rigid rotors and harmonic oscillator models based on the solution of their Schrödinger equation.	S4
2.5	Solve the Schrödinger equation for the hydrogen like elements.	S7
3	**Competence:**	
3.1	Manage resources, time and collaborate with members of the group.	C1
3.2	Work effectively both in a team, and independently on solving chemistry problems.	C2
3.3	Communicate effectively with his lecturer and colleagues	C1
3.4	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.	4
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
11	Overlap Matrix- Correlation Diagrams.	2
12	Revision	2
Total		30

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**		
1.1	List the historical development of the Origins of quantum theory	Lecture and web based study	quiz
1.2	Illustrate, qualitatively and quantitatively, the role of photons in understanding phenomena like the photoelectric effect and Compton scattering.	Lecture	quiz
1.3	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
1.4.	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.	Lecture	quiz
1.5	Define the concepts of spin and angular momentum, as well as their quantization-	Lecture	exam

Code	Course Learning Outcomes	Teaching Strategies	Assessment Methods
	and addition rules.		
1.6	Explain physical properties of atoms and molecules based on quantum Chemical formulations.	discussion	quiz
1.7	Describe a Qualitative treatment of the LCAO-MO for homonuclear and heteronuclear diatomic molecules as a well as Simple Hückel Molecular Orbital theory.	Lecture	quiz
2.0	**Skills**		
2.1	Give concise physical interpretations and discussions of quantum mechanics postulations in molecular orbitals treatment.	lecture	quiz
2.2	Solve the Schrödinger equation for simple one-dimensional systems and conclude the probabilities, Eigen and expectation values for these systems.	lecture	exam
2.3	Apply the particle-in-a-box model to π electrons in conjugated molecules.	lecture	quiz
2.4	Compare between the different energies of the rigid rotors and harmonic oscillator models based on the solution of their Schrödinger equation.	lecture	exam
2.5	Solve the Schrödinger equation for the hydrogen like elements.	lecture	exam
3.0	**Competence**		
3.1	Manage resources, time and collaborate with members of the group.	presentation	Observation of group's team work performance
3.2	Use university library and web search engines for collecting information and search about different topics.	project	Write a report
3.3	Work effectively both in a team, and independently on solving chemistry problems.	group discussion	Observation of group's team work performance
3.4	Communicate effectively with his lecturer and colleagues	group discussion	Observation by the instructor
3.5	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	Homework or activities.	--	10 %
2	First Periodic Exam.	8	20 %
3	Second Periodic Exam.	14	20 %

#	Assessment task*	Week Due	Percentage of Total Assessment Score
4	Final Exam.(2 hours exam)	16	50 %
5	**Total**		100%

***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 oflearning 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	

Received by: Dr. Ismail Althagafi **Department Head**

Signature: **Date: 20/12/2019**