

Kingdom of Saudi Arabia

The National Commission for

Academic Accreditation & Assessment



Course Specifications

Quantum Chemistry

402253

Institution: Umm Al-qura University	Date of Report: 2015
College/Department : Faculty of Applied Science/ Department of chemistry	

A. Course Identification and General Information

1. Course title and code: Quantum Chemistry/402253			
2. Credit hours: 2 hours			
3. Program(s) in which the course is offered. Chemistry program			
4. Name of faculty member responsible for the course: Dr Ahmed El Defrawy			
5. Level/year at which this course is offered: 4rd level/2st year			
6. Pre-requisites for this course (if any): 402121			
7. Co-requisites for this course (if any) -			
8. Location if not on main campus: both in El-Abdyah(boys side) and El-Zaher (girls side)			
9. Mode of Instruction (mark all that apply)			
a. Traditional classroom	<input checked="" type="checkbox"/>	What percentage?	<input type="text" value="80%"/>
b. Blended (traditional and online)	<input type="checkbox"/>	What percentage?	<input type="text"/>
c. e-learning	<input checked="" type="checkbox"/>	What percentage?	<input type="text" value="20%"/>
d. Correspondence	<input type="checkbox"/>	What percentage?	<input type="text"/>
f. Other	<input type="checkbox"/>	What percentage?	<input type="text"/>
Comments:			

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B Objectives

<p>1. What is the main purpose for this course?</p> <p>By the end of this course the students will be able to:</p> <ol style="list-style-type: none"> 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
<p>2. Briefly describe any plans for developing and improving the course that are being implemented. (e.g. increased use of IT or web based reference material, changes in content as a result of new research in the field)</p> <ol style="list-style-type: none"> 1. Computer labs to be used in teaching the student the basics of the application of the quantum chemistry soft ware used in the simulation, molecular modeling and quantum chemical calculations. 2. encourage students to make reports in the recent trends in the field of quantum chemistry, either from the library or by using the Internet.

C. Course Description (Note: General description in the form to be used for the Bulletin or handbook should be attached)

1. Topics to be Covered		
List of Topics	No. of Weeks	Contact Hours
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.	2	4
Operators and its Importance in Quantum Chemistry - Eigen Functions and Eigen Values	1	2
Schrödinger Equation Of Hydrogen Atom- Wave Function Equation and Energy	1	2
Different Quantum Numbers and their Uses in Describing the Orbitals and the Energy Levels.	1	2
Quantum Theory and Molecular Structure – Born-Oppenheimer Approximation.	1	2
revision	1	2
Molecular Orbital Theory and Molecular Structure-	1	2
Linear Combination of Atomic Orbitals (LCAO).	1	2
Application of Molecular Orbital Theory on Homonuclear Molecules.	1	2

Application of Molecular Orbital Theory on Heteronuclear Molecules	1	2
Overlap Matrix- Correlation Diagrams.	1	2
Practical Applications on Computational Software - Analysis and Discussion of the Results.	2	4
Revision	1	2

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2. Course components (total contact hours and credits per semester):						
	Lecture	Tutorial	Laboratory	Practical	Other:	Total
Contact Hours	32	-	-	-	-	32
Credit	2	-	-	-	-	2

3. Additional private study/learning hours expected for students per week.	-
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4. Course Learning Outcomes in NQF Domains of Learning and Alignment with Assessment Methods and Teaching Strategy
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	NQF Learning Domains And Course Learning Outcomes	Course Teaching Strategies	Course Assessment Methods
1.0	Knowledge		
1.1	List the historical development of the Origins of quantum theory	1.Lectures using white board and data show 2. Problem classes 3. discussion groups	1.Midterm exam 2.quizzes 3.Group discussion 4.Final exam
1.2	Illustrate, qualitatively and quantitatively, the role of photons in understanding phenomena like the photoelectric effect and Compton scattering.		
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).		
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.		
1.5	define the concepts of spin and angular momentum, as well as their quantization- and addition rules.		
1.	Explain physical properties of atoms and molecules		

6	based on quantum Chemical formulations.		
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.		
2.0	Cognitive Skills		
2. 1	Give concise physical interpretations and discussions of quantum mechanics postulations in molecular orbitals treatment.	1. group discussions 2. case study. 3. home work assignment containing problem thinking activities	1.Midterm exam 2.quizzes 3.Group discussion 4.Final exam
2. 2	solve the Schrödinger equation for simple one-dimensional systems and conclude the probabilities, Eigen and expectation values for these systems.		
2. 3	compare between the different energies of the rigid rotors and harmonic oscillator models based on the solution of their Schrödinger equation.		
2. 4	Solve the Schrödinger equation for the hydrogen like elements.		
3.0	Interpersonal Skills & Responsibility		
3. 1	Manage resources, time and collaborate with members of the group.	1. Team work groups for cooperative work making. 2. Presenting the analysis and interpretation of a case study for each group to the other groups in class. 3.Open a general discussion with students in the area of educational issues for knowledge transfer between the students.	1.Writing group scientific report for a case study. 2.Assessment of the solution of problems submitted by the students.
3. 2	Use university library and web search engines for collecting information and search about different topics .		
4.0	Communication, Information Technology, Numerical		
4. 1	Work effectively both in a team, and independently on solving chemistry problems.	1.Write a Report 2.Use digital libraries and/or E-Learning Systems for the communication with lecturer through the course work	1.Evaluating the activities of the students through the semester for their activities on the E-learning system, as well as, their communication with each other in different tasks.
4. 2	Communicate effectively with his lecturer and colleagues		
4. 3	Use IT and web search engines for collecting information.		

			2.Evaluation of the report presented
5.0	Psychomotor		
5.1	NOT APPLICABLE		

5. Schedule of Assessment Tasks for Students During the Semester			
	Assessment task (e.g. essay, test, group project, examination, speech, oral presentation, etc.)	Week Due	Proportion of Total Assessment
1	problem sets and case study	weekly	3%
2	Quizzes	To be assigned	3%
3	class test 1	7	20%
4	class test 2	13	20%
5	project	14	4%
6	Final exam	16	50%

D. Student Academic Counseling and Support

1. Arrangements for availability of faculty and teaching staff for individual student consultations and academic advice. (include amount of time teaching staff are expected to be available each week)
<ul style="list-style-type: none"> We have faculty members to provide counseling and academic advice. 2 hours per week as office hours are available for discussion with the students.

E. Learning Resources

1. List Required Textbooks I.N. Levine, Quantum chemistry, 6 rd edition, Allyn & Bacon, Inc. 1993. J. P. Lowe, quantum Chemistry, Academic press, New York, 1978.
2. List Essential References Materials (Journals, Reports, etc.) journal of Molecular Structure (Elsevier)
3. List Recommended Textbooks and Reference Material (Journals, Reports, etc) P.W. Atkins, Molecular quantum mechanics, oxford University press, New York, 1970. M.W. Hanna, Quantum mechanics in Chemistry, 5 th Edition, Benjamin, Menlo Park, California, 1988.
4. List Electronic Materials (eg. Web Sites, Social Media, Blackboard, etc.) <ul style="list-style-type: none"> http://en.wikipedia.org/wiki/ http://www.chemweb.com/

- Websites on the internet relevant to the topics of the course

5. Other learning material such as computer-based programs/CD, professional standards or regulations and software.

Hyperchem or Spartan software will be helpful beside some free software.

F. Facilities Required

Indicate requirements for the course including size of classrooms and laboratories (i.e. number of seats in classrooms and laboratories, extent of computer access etc.)

1. Accommodation (Classrooms, laboratories, demonstration rooms/labs, etc.)

Appropriate teaching class including white board and data show with at least 25 seats.

2. Computing resources (AV, data show, Smart Board, software, etc.)

Computer Halls access for the students will be helpful in doing their tasks during the course.

3. Other resources (specify, e.g. if specific laboratory equipment is required, list requirements or attach list)

Computational software will be helpful such as Spartan or hyperchem program packages.

G Course Evaluation and Improvement Processes

1 Strategies for Obtaining Student Feedback on Effectiveness of Teaching

- Student discussion with the instructor allow for continuous feedback through the course progress.
- Student Evaluation Questionnaires.

2 Other Strategies for Evaluation of Teaching by the Program/Department Instructor

- Discussions within the group of faculty teaching the course.
- Peer consultation on teaching strategies and its effectiveness.

3 Processes for Improvement of Teaching

- Workshops given by experts on new teaching and learning methodologies will be attended.
- Improving of the teaching strategies by monitoring the evaluation of the students progress through the semester

4. Processes for Verifying Standards of Student Achievement (e.g. check marking by an independent member teaching staff of a sample of student work, periodic exchange and remarking of tests or a sample of assignments with staff at another institution)

Not effective yet.

5 Describe the planning arrangements for periodically reviewing course effectiveness and planning for improvement.

- The course will be evaluated periodically after each semester based on the results of the students and the report presented by the teaching staff that will be discussed with the course coordinator so as to improve the course.

Faculty or Teaching Staff: Ahmed Mohamed El Defrawy

Signature:

Date Report Completed: 2015

Received by: Dr Hatem Altass Head of the Department

Signature: _____ **Date:** _____

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