

## COURSE SPECIFICATIONS Form

Course Title: **Quantum Chemistry**

Course Code: **4026822-3**



Date: 25-10-2018

Institution: Umm Al-Qura University.

College: Faculty of Applied Science

Department: Department of Chemistry

### A. Course Identification and General Information

1. Course title and code: **Quantum Chemistry / 4026822-3**

2. Credit hours: **3 ( theoretical)**

3. Program(s) in which the course is offered. **M. Sc. in Chemistry**

(If general elective available in many programs indicate this rather than list programs)

4. Name of faculty member responsible for the course. **Dr. Jaber El Fahemi**

5. Level/year at which this course is offered: **2<sup>nd</sup> / 1<sup>st</sup>**

6. Pre-requisites for this course (if any): --

7. Co-requisites for this course (if any): --

8. Location if not on main campus: **El-Abedyah, El-Azizya, and El-Zaher**

9. Mode of Instruction (mark all that apply):

a. Traditional classroom

percentage?

b. Blended (traditional and online)

percentage?

90

c. E-learning

percentage?

d. Correspondence

percentage?

f. Other

percentage?

10

Comments:

## B Objectives

### 1. The main objective of this course

The goal of course is to provide those post graduate students in chemistry with basic knowledge of quantum chemistry and interest in working in the fields of computational and theoretical chemistry with wave function based methods and their origin in fundamental quantum mechanics.

2. Describe briefly any plans for developing and improving the course that are being implemented. (e.g. increased use of the IT or online reference material, changes in content as a result of new research in the field)

- Updating the course content with the techniques that will be recently introduced in the field.
- The use of smart teaching halls for lectures.
- Increased use of IT or web based reference material.
- Encourage students to carry out research reports in the subjects using the library, data base services, and/or websites.

**C. Course Description** (Note: General description in the form used in the program's bulletin or handbook)

### Course Description:

#### 1. Topics to be Covered

List of Topics	No. of Weeks	Contact hours
Many-electron quantum mechanics	2	6
Exact and approximate wave functions	2	6
Solution of the Hartree–Fock equations	2	6
Configuration interaction	2	6
Coupled-cluster theory	1	3
Basis sets and molecular integrals	2	6
Numerical benchmarking of electronic-structure models	2	6

#### 2. Course components (total contact and credit hours per semester):

		Lecture	Tutorial	Laboratory/ Studio	Practical	Other	Total
Contact Hours	Planned	39	-	-	-	-	39
	Actual	39	-	-	-	-	39
Credit	Planned	3	-	-	-	-	3
	Actual	3	-	-	-	-	3

**3. Individual study/learning hours expected for students per week.**

**4. Course Learning Outcomes in NQF Domains of Learning and Alignment with Assessment Methods and Teaching Strategies**

On the table below are the five NQF Learning Domains, numbered in the left column.

**First**, insert the suitable and measurable course learning outcomes required in the appropriate learning domains (see suggestions below the table). **Second**, insert supporting teaching strategies that fit and align with the assessment methods and targeted learning outcomes. **Third**, insert appropriate assessment methods that accurately measure and evaluate the learning outcome. Each course learning outcomes, assessment method, and teaching strategy should fit in together with the rest to form an integrated learning and teaching process. (Courses are not required to include learning outcomes from each domain.)

**Curriculum Map**

Code #	NQF Learning Domains And Course Learning Outcomes	Course Teaching Strategies	Course Assessment Methods
<b>1.0</b>	<b>Knowledge</b>		
1.1	Recognize the central aspects of the quantum-chemical methods for molecules	<ul style="list-style-type: none"> <li>• Use of the internet to carry out some reports on course subjects.</li> <li>• Lectures</li> <li>• Discussion groups</li> <li>• Seminar</li> <li>• In class problems</li> </ul>	<ul style="list-style-type: none"> <li>• Written assignments</li> <li>• Presentations</li> <li>• Formal mid-term and final exams.</li> </ul>
1.2	Account for the basic principles behind some methods that combine quantum mechanics and classical force fields.		
1.3	Differentiate between the advantages and disadvantages of the various methods discussed in the course.		
1.4	Describe some of the important and timely current problems within the area of quantum chemistry methods and calculations internationally.		
<b>2.0</b>	<b>Cognitive Skills</b>		
2.1	Use some of these models and methods in practical quantum-chemical calculations.	<ul style="list-style-type: none"> <li>• Web-based study.</li> <li>• Lectures.</li> <li>• Scientific discussion</li> <li>• Library visits.</li> </ul>	<ul style="list-style-type: none"> <li>• Measuring the response to the assignments.</li> <li>• Periodic tests and assignments.</li> </ul>
2.2	Predict the different electronic wave functions.		
2.3	Explain the contents of Density Functional Theory and correlated methods like Configuration Interaction, Møller Plesset Perturbation Theory and Coupled Cluster.		
2.4	Apply perturbation theory in the calculation of different properties of atoms and molecules.		
<b>3.0</b>	<b>Interpersonal Skills &amp; Responsibility</b>		
3.1	Manage resources, time and collaborate with members of the group	<ul style="list-style-type: none"> <li>• Teamwork groups for cooperative work making.</li> <li>• Solving problems in groups during lecture.</li> </ul>	<ul style="list-style-type: none"> <li>• Oral presentations</li> <li>• Group discussion</li> <li>• Reports</li> </ul>
3.2	Use university library and web search engines for		

	collecting information and search about different topics	<ul style="list-style-type: none"> <li>Open discussion about recent topic of the course</li> </ul>	
<b>4.0</b>	<b>Communication, Information Technology, Numerical</b>		
4.1	Work effectively both in a team, and independently on solving chemistry problems.	<ul style="list-style-type: none"> <li>Use digital libraries for literature survey</li> <li>Use E-Learning Systems for the communication with lecturer through the course work</li> </ul>	<ul style="list-style-type: none"> <li>Web-based student performance systems.</li> <li>Individual and group presentations.</li> <li>Evaluating the activities of the students through the semester .</li> </ul>
4.2	Communicate effectively with his lecturer and colleagues		
4.3	Use information and communication technologies		
<b>5.0</b>	<b>Psychomotor(if any)</b>		
5.1	Not applicable		

#### 5. Assessment Task Schedule for Students During the Semester

	Assessment task (i.e., essay, test, quizzes, group project, examination, speech, oral presentation, etc.)	Week Due	Proportion of Total Assessment
1	Assignments and activities.	--	10 %
2	Midterm Exam.	8	30 %
3	Final Exam.	15-16	60 %
4	Total		100%

#### D. Student Academic Counseling and Support

1. Arrangements for availability of faculty and teaching staff for individual student consultations and academic counseling. (include the time teaching staff are expected to be available per week)
  - Availability of Staff members to provide counselling and advice.
  - Office hours: During the working hours weekly.
  - Academic advising for students.

#### E Learning Resources

##### 1. List Required Textbooks

- T. Helgaker, P. Jørgensen, and J. Olsen, (2013). Molecular Electronic Structure Theory, Wiley, 1 edition.
- Kong Wan, Quantum Mechanics: A Fundamental Approach, 1<sup>st</sup> ed., CRC press, 2019.

##### 2. List Essential References Materials (Journals, Reports, etc.)

- Lecture hand outs available on the coordinator website.

##### 3. List Electronic Materials, Web Sites, Facebook, Twitter, etc.

- <http://en.wikipedia.org/wiki/>
- <http://www.chemweb.com/>
- Websites on the internet relevant to the topics of the course

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

- Computational chemistry software packages will be considered whenever appropriate.

## 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. **Technology 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 hyperchem program package.

## G Course Evaluation and Improvement Procedures

1. **Strategies for Obtaining Student's 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 Instructor or the Department**

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

3. **Procedures for Teaching Development**

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

- Peer reviewing of random samples including periodic and final exams of the students will be done.

**5. Describe the planning arrangements for periodically reviewing course effectiveness and planning for developing it.**

- 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 to improve the course.

**Name of Course Instructor: Dr. Jaber El Fahemi**

Signature  Date Completed: 25 – 10 - 2018

**Program Coordinator: Dr. Ismail Ibrahim Althagafi**

Signature:  Date Received: 27/10/2018

