ATTACHMENT 5.

Kingdom of Saudi Arabia

The National Commission for Academic Accreditation & Assessment

T6. Course Specifications

(CS)

Quantum Chemistry

(402642-3)

Course Specifications

Institution: **Umm Al-qura University**	Date: **2017**
College/Department: **Faculty of Applied Sciences / Department of Chemistry**	

A. Course Identification and General Information

1. Course title and code: Quantum Chemistry / **402642–3**			
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: **2nd / 1st**			
6. Pre-requisites for this course (if any): **not applicable**			
7. Co-requisites for this course (if any): **not applicable**			
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		What percentage?	
b. blended (traditional and online)	√	What percentage?	80
c. e-learning	√	What percentage?	10
d. correspondence		What percentage?	
f. other	√	What percentage?	10
Comments:			

B Objectives

1. What is the main purpose for 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. 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)

- Increasing the use of E-learning.
- Updating the course content with the techniques that will be recently introduced in the field.

C. Course Description (Note: General description in the form used in 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 hours and credits per semester):

	Lecture	Tutorial	Laboratory or Studio	Practical	Other:	Total
Contact Hours	**39**					**39**
Credit	**3**					**3**

3. Additional private study/learning hours expected for students per week.	2 hours

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

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 intended learning outcomes. **Third**, insert appropriate assessment methods that accurately measure and evaluate the learning outcome. Each course learning outcomes, assessment method, and teaching strategy ought to reasonably fit and flow together as an integrated learning and teaching process. (Courses are not required to include learning outcomes from each domain.)

Code #	**NQF Learning Domains And Course Learning Outcomes**	**Course Teaching Strategies**	**Course Assessment Methods**
1.0	**Knowledge**		
1.1	Recognize the central aspects of the quantum-chemical methods for molecules	• Traditional lectures • Seminar • In class problems • Discussion groups	• Written assignments • Presentations • Formal exams
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.		
2.0	**Cognitive Skills**		
2.1	Use some of these models and methods in practical quantum-chemical calculations.	• In class problems • Discussion groups	• Written assignments • Formal exams
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.		
3.0	**Interpersonal Skills & Responsibility**		
3.1	Manage resources, time and collaborate with members of the group	• Teamwork groups for cooperative work making. • Presentations	• Oral presentations • Group discussion
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.	• Use digital libraries for literature survey • Use E-Learning Systems for the communication with	• Evaluating the activities of the students through the semester for
4.2	Communicate effectively with his lecturer and colleagues		

4.3	Use IT and web search engines for collecting information.	lecturer through the course work	their activities on the E-learning. Evaluation of the literature surveys presented
5.0	**Psychomotor**		
5.1	Not Applicable.		
5.2			

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	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 advice. (include amount of time teaching staff are expected to be available each week)

- We have faculty members to provide consulting and academic advice.
- 2 hours per week as office hours are available for discussion with the students.

E Learning Resources

1. List Required Textbooks

- T. Helgaker, P. Jørgensen, and J. Olsen, (2013). Molecular Electronic Structure

Theory, Wiley, 1 edition. • R. McWeeny, (1992). Methods for Molecular Quantum Mechanics, Academic Press.
2. List Essential References Materials (Journals, Reports, etc.) International Journal of Quantum Chemistry Journal of Molecular Modeling
3. List Recommended Textbooks and Reference Material (Journals, Reports, etc) Any other journals in the field of quantum chemistry will be considered.
4. List Electronic Materials, Web Sites, Facebook, Twitter, etc. www.elsiver.com www.springer.com www.wiley.com
5. 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. 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 hyperchem program package.

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 Instructor or by the Department • 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) • 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 improvement. • The course will be evaluated periodically after each semester based on the results of the students and the report presented by the teaching stuff that will be discussed with the course coordinator to improve the course.

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

Signature:_____Date Report Completed:_____

Name of Field Experience Teaching Staff _____

Program Coordinator:_____

Signature: _____ Date Received:_____