

**ATTACHMENT 5.**

**Kingdom of Saudi Arabia**  
**The National Commission for Academic Accreditation &  
Assessment**

**T6. Course Specifications**  
**(CS)**

**Computational Chemistry**

**(402741-2)**



## Course Specifications

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

### A. Course Identification and General Information

1. Course title and code: <b>Computational Chemistry / 402741-2</b>	
2. Credit hours <b>2 hrs (theoretical)</b>	
3. Program(s) in which the course is offered: <b>Ph. D. in Chemistry</b>	
4. Name of faculty member responsible for the course: <b>Dr. Jabir Al-Fahemi</b>	
5. Level/year at which this course is offered: <b>1<sup>st</sup> / 1<sup>st</sup></b>	
6. Pre-requisites for this course (if any): <b>not applicable</b>	
7. Co-requisites for this course (if any): <b>not applicable</b>	
8. Location if not on main campus: <b>El-Abedyah, El-Azizya, and El-Zaher</b>	
9. Mode of Instruction (mark all that apply)	
a. traditional classroom	<input type="checkbox"/> What percentage? <input type="checkbox"/>
b. blended (traditional and online)	<input checked="" type="checkbox"/> What percentage? <input type="checkbox"/> 80
c. e-learning	<input checked="" type="checkbox"/> What percentage? <input type="checkbox"/> 10
d. correspondence	<input type="checkbox"/> What percentage? <input type="checkbox"/>
f. other	<input checked="" type="checkbox"/> What percentage? <input type="checkbox"/> 10
Comments:	

## B Objectives

### 1. What is the main purpose for this course?

The first goal of the module is to achieve a sufficient understanding of the theory behind computational chemistry and give students a sound appreciation of the many ways in which computational chemistry can be used to solve chemical problems. The second goal is to employ several programs (such as Gaussian, MOPAC and HyberChem) to calculate the structures and properties of molecules and solids.

### 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):

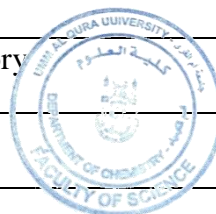
The students will be mentioned to prepare an essay or a report from literature using the library, data base services, and/or websites to follow up and update the new topics of the subject of the course

## C. Course Description (Note: General description in the form used in Bulletin or handbook)

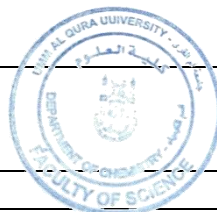
Course Description:

### 1. Topics to be Covered

List of Topics	No. of Weeks	Contact hours
What are theory, computation, and modeling	1	2
Molecular mechanics	1	2
Simulations of molecular ensembles	1	2
Foundations of molecular orbital theory	1	2
Semiempirical implementations of molecular orbital theory	3	6
Applications using software	1	2



Ab Initio implementations of Hartree-Fockmolecular orbital theory	2	4
Density functional theory	3	6



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

	Lecture	Tutorial	Laboratory or Studio	Practical	Other:	Total
Contact Hours	26					26
Credit	2					2

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

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	By the end of this course student will be able to understand theories of computational	<ul style="list-style-type: none"> <li>• Traditional lectures</li> <li>• Seminar</li> </ul>	<ul style="list-style-type: none"> <li>• Written assignments</li> </ul>

	chemistry and recognize its importance in solving chemical problems.	<ul style="list-style-type: none"> <li>• In class problems</li> <li>• Discussion groups</li> </ul>	<ul style="list-style-type: none"> <li>• Presentations</li> <li>• Formal exams</li> </ul>
1.2			
2.0	Cognitive Skills		
2.1	By the end of this course students will be able to apply various chemical software to calculate structures and properties of molecules.		
2.2			
3.0	Interpersonal Skills & Responsibility		
3.1	<ul style="list-style-type: none"> <li>• Take the personality and responsibility for their own learning.</li> </ul>	<ul style="list-style-type: none"> <li>• Teamwork groups for cooperative work making.</li> <li>• Presentations</li> </ul>	<ul style="list-style-type: none"> <li>• Oral presentations</li> <li>• Group discussion</li> </ul>
3.2	<ul style="list-style-type: none"> <li>• Working effectively in groups and exercise leadership when appropriate.</li> </ul>		
	<ul style="list-style-type: none"> <li>• Act ethically and consistently with high molar standards in personal and public fourm.</li> </ul>		
	Community linked thinking		
4.0	Communication, Information Technology, Numerical		
4.1	<ul style="list-style-type: none"> <li>• Communicate effectively in oral and written forms.</li> </ul>	<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>• Evaluating the activities of the students through the semester for their activities on the E-learning.</li> </ul>
4.2	<ul style="list-style-type: none"> <li>• Use information and communication technologies.</li> </ul>		
4.3	<ul style="list-style-type: none"> <li>• Use basic mathematical and statistical techniques</li> </ul>		

5.0	Psychomotor		
5.1			
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	<b>Total</b>		<b>100 %</b>

#### 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 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

1- Essentials of Computational Chemistry: Theories and models, Christopher J Cramer, WILEY, 2004.

2- Introduction to Computational Chemistry, Frank Jensen, WILEY, 2007.

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 computational chemistry will be considered.

4. List Electronic Materials, Web Sites, Facebook, Twitter, etc.

[www.elsiver.com](http://www.elsiver.com)

[www.springer.com](http://www.springer.com)

[www.wiley.com](http://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.

<ul style="list-style-type: none"><li>Improving of the teaching strategies by monitoring the evaluation of the students progress through the semester</li></ul>
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) <ul style="list-style-type: none"><li>Peer reviewing of random samples including periodic and final exams of the students will be done.</li></ul>
5 Describe the planning arrangements for periodically reviewing course effectiveness and planning for improvement. <ul style="list-style-type: none"><li>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.</li></ul>

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

Signature: \_\_\_\_\_ Date Report Completed: \_\_\_\_\_

Name of Field Experience Teaching Staff \_\_\_\_\_

Program Coordinator: \_\_\_\_\_

Signature: \_\_\_\_\_ Date Received: \_\_\_\_\_

