Kingdom of Saudi Arabia

The National Commission for

Academic Accreditation & Assessment

COURSE SPECIFICATION

(Quantum Chemistry, 402353-2)

1435 / 1436 H

Course Specification

Institution: **Umm Al-Qura University**
College/Department: **Faculty of Applied Sciences / Chemistry Department**

A. Course Identification and General Information

1. Course title and code: **Quantum Chemistry 4, 402353-2**
2. Credit hours: **2 h (theoretical)**
3. Program(s) in which the course is offered. (If general elective available in many programs indicate this rather than list programs) **Pure Chemistry**
4. Name of faculty member responsible for the course: **Dr. Ahmed Mohamed El Defrawy**
5. Level / year at which this course is offered: **5th level / 3**
6. Pre-requisites for this course (if any): **General Chemistry, 402101-4**
7. Co-requisites for this course (if any): ——
8. Location if not on main campus: ——

B. Objectives

1. Summary of the main learning outcomes for students enrolled in the course. By the end of this course the students will be able to: • describe the fundamental principles of quantum chemistry. • state the fundamental postulates of quantum mechanics. • develop physical intuition, mathematical reasoning, and problem solving skills. • study the solution of Schrodinger equation for some simple systems. • be further prepared for the necessarily rigorous sequence in chemistry courses needed the quantum chemistry.
2. **Briefly describe any plans for developing and improving the course** that are being implemented. (eg increased use of IT or web based reference material, changes in content as a result of new research in the field) • Computer hall 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.

- Using the facilities offered by the university in E-learning for communication with the students.

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		
Topic	No of Weeks	Contact hours
Origins of quantum theory, wave-particle duality and postulates of quantum mechanics	2	4
Schrödinger Equation, quantum mechanical operators and Eigen value Equations	2	4
Wave functions and Probability and expectation Values , Free particle and Particle-in a one, two and three dimensional box.	1	2
Heisenberg Uncertainty Principle	1	2
Qualitative treatment of simple harmonic oscillator model of vibrational motion	1	2
Angular momentum	1	2
Rigid rotator model of rotation of diatomic molecule	1	2
Qualitative treatment of hydrogen atom and hydrogen-like ions.	1	2
Schrödinger equation for many-electron atoms.	1	2
The Born-Oppenheimer approximation, Variation theorem and application to simple systems.	1	2
Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules.	1	2
Simple Hückel Molecular Orbital (HMO) theory and its application to simple polyenes (ethene, butadiene).	1	2

2. Course components (total contact hours per semester):			
Lecture: **28**	Tutorial:	Practical/Fieldwork/Internship:	Other:

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

(This should be an average: for the semester not a specific requirement in each week)

- Two office hours per weak.

4. Development of Learning Outcomes in Domains of Learning

For each of the domains of learning shown below indicate:

- A brief summary of the knowledge or skill the course is intended to develop;
- A description of the teaching strategies to be used in the course to develop that knowledge or skill;
- The methods of student assessment to be used in the course to evaluate learning outcomes in the domain concerned.

a. Knowledge

(i) Description of the knowledge to be acquired

By the end of this course the student will be able to:

- List the historical development of the Origins of quantum theory
- Illustrate, qualitatively and quantitatively, the role of photons in understanding phenomena like the photoelectric effect and Compton scattering.
- 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).
- 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.
- Define the concepts of spin and angular momentum, as well as their quantization- and addition rules.
- Explain physical properties of atoms and molecules based on quantum Chemical formulations.
- Describe a qualitative treatment of the LCAO-MO for homonuclear and heteronuclear diatomic molecules as a well as Simple Hückel Molecular Orbital theory.

(ii) Teaching strategies to be used to develop that knowledge

- Lectures using white board and data show.
- Problem classes.
- Discussion groups.

(iii) Methods of assessment of knowledge acquired

- Midterm exam
- quizzes
- Group discussion
- Final exam.

b. Cognitive Skills

(i) Cognitive skills to be developed

By the end of the course the student will be able to:

- Give concise physical interpretations and discussions of quantum mechanics postulations in molecular orbitals treatment.
- Solve the Schrödinger equation for simple one-dimensional systems and conclude the probabilities, Eigen and expectation values for these systems.
- Compare between the different energies of the rigid rotors and harmonic oscillator models based on the solution of their Schrödinger equation.
- Solve the Schrödinger equation for the hydrogen like elements.

(ii) Teaching strategies to be used to develop these cognitive skills

- Group discussions.
- Case study.
- Home work assignment containing problem thinking activities.

(iii) Methods of assessment of students cognitive skills

- Midterm exam
- Quizzes
- Home work assignments.
- Group discussion
- Final exam

c. Interpersonal Skills and Responsibility

(i) Description of the interpersonal skills and capacity to carry responsibility to be developed

By the end this course, students will be able:

- Manage resources, time and collaborate with members of the group.

- Use university library and web search engines for collecting information and search about different topics.

(ii) Teaching strategies to be used to develop these skills and abilities

- Team work groups for cooperative work making.
- Presenting the analysis and interpretation of acase study for each group to the other groups in class.
- Open a general discussion with students in the area of educational issues for knowledge transfer between the students.

(iii) Methods of assessment of students interpersonal skills and capacity to carry responsibility

- Writing group scientific report for a case study.
- Assessment of the solution of problems submitted by the students.

d. Communication, Information Technology and Numerical Skills

(i) Description of the skills to be developed in this domain.

- Work effectively both in a team, and independently on solving chemistry problems.
- Communicate effectively with his lecturer and colleagues.
- Use IT and web search engines for collecting information.

(ii) Teaching strategies to be used to develop these skills

- Write a Report
- Use digital libraries and/or E-Learning Systems for the communication with lecturer through the course work.

(iii) Methods of assessment of students numerical and communication skills

- 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.
- Evaluation of the report presented.

e. Psychomotor Skills (if applicable)

(i) Description of the psychomotor skills to be developed and the level of performance required

- Not applicable in this course.

(ii) Teaching strategies to be used to develop these skills

- Not applicable in this course.

(iii) Methods of assessment of students psychomotor skills

- Not applicable in this course.

5. Schedule of Assessment Tasks for Students During the Semester:			
Assessment	**Assessment task (eg. essay, test, group project, examination etc.)**	**Week due**	**Proportion of Final Assessment**
1	Class activities, Attendances and Duties	Throughout the Term	**10%**
2	Mid-Term Exam (s)	5-14	**40%**
3	Final Exam	End of the Term	**50%**
4	**Total**		**100%**

D. Student Support

1. Arrangements for availability of faculty for individual student consultations and academic advice. (include amount of time faculty are available each week)

- 2 hours per week as office hours are available for discussion with the students.

E. Learning Resources

1. Required Text(s)

- Molecular Quantum Mechanics, Peter Atkins and Ronald Friedman, 4th ed., Oxford, University Press, 2005.
- Quantum Mechanics for chemists, David O. Hayward, RSC, 2002

2. Essential References

- Quantum Chemistry, Ira N. Levine, 6th ed., Allyn & Bacon Inc., 1993.

3- Recommended Books and Reference Material (Journals, Reports, etc) (Attach List)

- Quantum Chemistry, John P. Lowe, Academic Press, 1978.

4-.Electronic Materials, Web Sites etc

- 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/regulations • Quantum chemistry software such as hyperchem.

F. Facilities Required

Indicate requirements for the course including size of classrooms and laboratories (ie number of seats in classrooms and laboratories, extent of computer access etc.)
1. Accommodation (Lecture rooms, laboratories, etc.) • Appropriate teaching class including white board and data show with at least 25 seats.
2. Computing resources • Computer Lab access for the students will be helpful in doing their tasks during the course.
3. **Other resources** (specify --eg. If specific laboratory equipment is required, list requirements or attach list) • Hyperchem Computer software will be helpful beside some free software.

G. Course Evaluation and Improvement Processes

1. Strategies for Obtaining Student Feedback on Effectiveness of Teaching • Student discussion with the instructor allow for continuous feed back through the course progress. • Student Evaluation Surveys.
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 (eg. check marking by an independent faculty member of a sample of student work, periodic exchange and remarking of a sample of assignments with a faculty member in 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 stuff that will be discussed with the course coordinator so as to improve the course.