Course Specification

(Postgraduate Programs)

Course Title:	**Advanced Quantum**
Course Code:	**CHM 6247**
Program:	Master of science in chemistry
Department:	Chemistry
College:	Science
Institution:	Imam Mohammad Ibn Saud Islamic University
Version:	*Course Specification Version Number*
Last Revision Date:	*Pick Revision Date.*

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A. General information about the course:

1. Course Identification:

1. Credit hours: 3 (3 Lectures, 0 Lab, 0 Tutorials)				
2. Course type				
A.	☐University	☐College	☐Department	☐Track
B.	☐Required		☒ Elective	
3. Level/year at which this course is offered: Level 1/Year 2				

4. Course General Description:

This course deals with History of QM and postulates, Particle in the box, particle in three dimensional box, Basic operator algebra, Harmonic oscillator and rigid rotor, Vibrational and rotational spectroscopy. The hydrogen atom wave function (radial and angular parts), atomic orbitals. Many-electron atoms, Hartree-Fock, quantum states, term symbols, Atomic spectroscopy, The chemical bond, molecular orbital theory, Electronic spectroscopy. Approximation methods: perturbation Theory, variation theory, Pauli principle, Slater determinants. Computational chemistry cont., nuclear spins.

5. Pre-requirements for this course (if any):

Advanced Physical Chemistry – CHM 6141

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

None

7. Course Main Objective(s):

- **Improve their knowledge of the fundamentals and concepts of advanced quantum chemistry.**
- **Recognize the applications of Schrodinger Eq. For one electron atom and many electron atoms.**
- **Develop their knowledge of the Quantum mechanics and atomic molecular and electronic spectroscopy.**
- **Be familiar with Approximation methods: perturbation Theory.**
- **Identify Computational chemistry.**

2. Teaching Mode: (mark all that apply)

No	Mode of Instruction	Contact Hours	Percentage
1	Traditional classroom	45	100 %
2	E-learning		
3	Hybrid • Traditional classroom		

No	Mode of Instruction	Contact Hours	Percentage
	• E-learning		
4	Distance learning		

3. Contact Hours: (based on the academic semester)

No	Activity	Contact Hours
1.	**Lectures**	45
2.	**Laboratory/Studio**	0
3.	**Field**	0
4.	**Tutorial**	0
5.	**Others (specify)……**	0
	Total	45

B. Course Learning Outcomes (CLOs), Teaching Strategies and Assessment Methods:

Code	Course Learning Outcomes	Code of CLOs aligned with program	Teaching Strategies	Assessment Methods
1.0	**Knowledge and understanding**			
1.1	**To recall the basic operator algebra, Harmonic oscillator and rigid rotor, Vibrational and rotational spectroscopy. Recognize the principles of the particle in the box, particle in three-dimensional box.**	**K1. *Phy.*; K4. *Phy.***	▪ Five hours/week lectures. ▪ Self-study Home-exam.	▪ Regular Exams ▪ Assignments ▪ Short Quizzes ▪ Oral Discussion Participation.
1.2	**To describe the Structure and spectra of hydrogen atomic orbitals and Many-electron atoms, Hartree-Fock, quantum states,**	**K1. *Phy.*; K4. *Phy.***	▪ Five hours/week lectures. ▪ Think to justify the Characterization Techniques applications in	▪ Oral Discussion marks ▪ Literatures Survey ▪ Mini-seminar. ▪ Participation.

Code	Course Learning Outcomes	Code of CLOs aligned with program	Teaching Strategies	Assessment Methods
	Atomic spectroscopy, Electronic spectroscopy.		Atomic spectroscopy, using available references (SDL) online Open discussion.	
1.3	**To define the approximation methods.**	**K1. *Phy.*; K4. *Phy.***	▪ Five hours/week lectures. Group Discussion using available references (SDL) online.	▪ Midterm. ▪ Assignments. ▪ Group Discussions. ▪ Literatures Survey ▪ Mini-seminar. Participation.
1.4	**To recognize the application of Quantum mechanics and atomic molecular, and electronic spectroscopy.**	**K1. *Phy.*; K3.*Phy.*; K4. *Phy.***	▪ Five hours/week lectures Group Discussion on application of Quantum mechanics and atomic molecular, using available references (SDL) online.	▪ Assignments ▪ Open Discussions. ▪ Literatures Survey ▪ Mini-seminar. Participation.
2.0	**Skills**			
2.1	**To explain the concepts and principles of quantum chemistry.**	**S1. *Phy.*; S2.*Phy.***	▪ Lectures activity ▪ Self-study. Deep discussion on concepts and principles of quantum chemistry.	▪ Questions in Lectures. ▪ Short Quizzes and Exams. ▪ Open Discussions. ▪ Participation Mini –seminar.
2.2	**To analyze problems and explore strategies to calculate the energies of atomic orbital for hydrogen and hydrogen-like atoms and many - electron atoms.**	**S1. *Phy.*; S3.*Phy.***	▪ Practice some examples to calculate the energies of atomic orbital, achieving. ▪ Brainstorming. Self-study	▪ Questions in Lectures. ▪ Participation ▪ Oral Discussion Short Quizzes.
2.3	**To summarize Basic principles of Quantum**	**S1. *Phy.***	▪ Lectures ▪ Oral	▪ Questions in Lectures.

Code	Course Learning Outcomes	Code of CLOs aligned with program	Teaching Strategies	Assessment Methods
	mechanics and its Applications.		Discussions. ▪ Brainstorming. Self-study	▪ Short Quizzes and Exams. ▪ Oral Discussion. Participation.
2.4	**To operate communication to computational chemistry, and its applications in Quantum mechanics and atomic molecular, accompanying writing of mini- Reports, operating electronic mail, and Network in communicating with others.**	**S1. *Phy.*; K4. *Phy.***	▪ Group Discussion and Assignments. ▪ Suggest several examples of Computational chemistry, and its applications in Quantum mechanics, for reading, writing, and oral presentation in groups. Encourage students to use electronic mail to submit Home Exams and Assignments	▪ Oral Discussion. ▪ Quizzes, and Exams. ▪ Giving marks for Oral Discussion in Lectures. Marks given for Assignments
3.0	**Values, autonomy, and responsibility**			
3.1	**Perform a scientific presentation, research, and work independently and integrate with a collaborated group, Using IT to acquire, analyze, and communicate information.**	**V1.*Phy.***	▪ Brainstorming. ▪ Exercises ▪ Group Discussion. ▪ Team work.	▪ Oral Discussion. ▪ Group Discussion ▪ Assignments.

Code	Course Learning Outcomes	Code of CLOs aligned with program	Teaching Strategies	Assessment Methods
3.2	**To demonstrate his ability to the effectively collaboration effectively the collaboration and inter-professionalism in class discussions or team works, as well as independently.**	**V1. *Phy*.; V1. *Phy*.**	▪ Small Group tasks ▪ Open discussion at classroom. ▪ Office hour guiding. Group Presentation of mini-projects	▪ Participation ▪ Homework's Mini-project(s).

C. Course Content:

No	List of Topics	Contact Hours
1.	***Basic principles of Quantum mechanics (QM): Schrödinger equationand the postulates of QM. Applications of Quantum mechanics*:** Study the applications of QM on some simple systems and include the translational, vibration and rotation motions: the translational motions: motion of Particle in the box, motion of particle in three-dimensional box, Vibrational motion: include harmonic oscillator, rotational motion: include rigid rotor. Vibrational and rotational spectroscopy.	**16**
2.	***The hydrogen atom:*** Wave function of the hydrogen atom (radial and angular parts), atomic orbitals.	**6**
3.	***Many-electron atoms:*** Hartree-Fock method and Slater determinants, quantum states, term symbols, Atomic spectroscopy, the chemical bond, molecular orbital theory, Hückel method calculations to determine electron energies of molecular orbitals, Electronic spectroscopy.	**6**
4.	***Approximation methods in QM***: Perturbation Theory, variation theory.	**6**
5	***Pauli principle and nuclear spins.***	**4**
6	***Computational chemistry:*** Methods of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and properties of molecules and solids using ab initio and semi-empirical approaches.	**7**
Total		45

D. Students Assessment Activities:

No	Assessment Activities *	Assessment timing (in week no)	Percentage of Total Assessment Score
1.	Class Activities (Open Discussion, Mini-reports, Oral Presentation, solving questions)	weekly	30 %
2.	Midterm Exam	9th week	30 %
3.	Final Exam	17 th week	40 %
4.	Total		100%

*Assessment Activities (i.e., Written test, oral test, oral presentation, group project, essay, etc.)

E. Learning Resources and Facilities:

1. References and Learning Resources:

Essential References	***Quantum Chemistry and Spectroscopy.*** Engel, Th., Pearson, Boston, 3rd edition, 2013. ISBN-13: 978-0321766199 ***Molecular Quantum Chemistry***. Atkins, P. W.; Friedman, R. S. Oxford University Press, 5th ed. 2010. ISBN: 9780199541423. ***Quantum Chemistry***. Levine, I. N. , Pearson, Boston, 7th edition, 2013. ISBN-13: 978-0321803450
Supportive References	***Quantum Chemistry***, I. N. Levine, 7th Ed., Pearson, Boston, (2014), ISBN-13: 978-0321803450
Electronic Materials	Saudi Digital Library
Other Learning Materials	• Blackboard • Multimedia associated with the text book and the relevant websites.

3. Educational and Research Facilities and Equipment Required:

Items	Resources
facilities (Classrooms, laboratories, exhibition rooms, simulation rooms, etc.)	**Each of the classroom should be equipped with a whiteboard and a projector, with a maximum of 20 students.**
Technology equipment (projector, smart board, software)	**The rooms are equipped with data show, Smart Board, WI-FI access.**

Items	Resources
Other equipment (depending on the nature of the specialty)	**None**

F. Assessment of Course Quality:

Assessment Areas/Issues	Assessor	Assessment Methods
Effectiveness of teaching	Students	**Direct:** Questionnaire.
	Course Responsible	**Direct:** Course e-Portfolio. **Indirect:** Second examiner checklist-Course report.
	Peer Reviewer	**Direct:** Questionnaire. **Indirect:** External assessor report.
Effectiveness of students assessment	Program Leaders	**Direct:** Course e-Portfolio. **Indirect:** Course report.
Quality of learning resources	Students	**Indirect:** Second examiner checklist-Course report.
	Faculty (Academic Advisory-GCC)	**Direct:** course Entrance/Exit. **Indirect:** Observations - Accreditation review.
	Program Leaders	**Direct:** Course e-Portfolio. **Indirect:** Course evaluation survey- Observations- Syllabus review- Accreditation review.
	Course Responsible	
The extent to which CLOs have been achieved	Course Responsible	**Direct:** Exams - Course e-Portfolio. **Indirect:** Second examiner checklist-Course report.
	Program Leaders	**Indirect:** Exams.
Other		

Assessor (Students, Faculty, Program Leaders, Peer Reviewer, Others (specify)
Assessment Methods (Direct, Indirect)

G. Specification Approval Data:

COUNCIL /COMMITTEE	Council of Chemistry Department
REFERENCE NO.	10 (No. 2/10)
DATE	21/04/1444- 15/11/2022