Course Syllabus

1	**Course title**	Quantum Chemistry
2	**Course number**	0333741
3	**Credit hours**	3 Hours
	Contact hours (theory, practical)	(3,0)
4	**Prerequisites / corequisites**	0303342, 0301221
5	**Program title**	Master of Science in Chemistry
6	**Program code**	0303
7	**Awarding institution**	The University of Jordan
8	**School**	Science
9	**Department**	Chemistry
10	**Course level**	Postgraduate/Master
11	**Year of study and semester (s)**	First or second year, Fall or Spring semesters
12	**Other department(s) involved in teaching the course**	N/A
13	**Main teaching language**	English
14	**Delivery method**	☒ Face to face learning ☐ Blended ☐ Fully online
15	**Online platforms(s)**	☐ Moodle ☒ Microsoft Teams ☐ Skype ☐Zoom ☐Others……
16	**Issuing/Revision Date**	October 15-2023

17 Course Coordinator:

Name: Wissam Helal	Contact hours: S, T, T: 10:30 – 12:30
Office number: Chemistry extension building	Phone number: 22175
Email: wissam.helal@ju.edu.jo	

18 Other instructors:

N/A

19 Course Description:

Quantum chemistry, intended for postgraduates majoring in chemistry, explore advanced concepts and ideas of quantum mechanics, quantum chemistry, atomic structure and spectroscopy, molecular structure and spectroscopy, and basic electronic structure theory. The course covers theorems and postulates of quantum mechanics; systems with exact solutions of Schrodinger equation, including the hydrogen atom; approximation methods (variational and perturbation theories); electronic structure of atoms and atomic term symbols, electronic structure of diatomic molecules; and an introduction to Hartree-Fock theory.

20 Course aims and outcomes:

A- Aims:

1. Develop a solid understanding of the fundamental principles of quantum chemistry.

2. Explain the fundamental concepts of and language of quantum chemistry.
3. Acquire a quantitative understanding of quantum chemistry, by both expressing concepts into mathematical relations, and by understanding physical concepts behind mathematical formulas. Furthermore, students will be able to derive important mathematical relations.
4. Promote problem-solving skills by applying different mathematical methods and techniques to the solution of relevant, but relatively complex, problems.
5. Appreciate the continuous interplay between experiment and theory in quantum chemistry.

B- Course Learning Outcomes (CLOs): Upon successful completion of this course students will be able to:

CLO-1. Acquire fundamental conceptual way of thinking related to atomic and molecular structure.
CLO-2. Apply problem solving skills to solve chemical problems using quantum chemistry methods.
CLO-3. Gain working experience with different computational chemistry tools.

21. Topic Outline and Schedule:

Week	Lecture	Topic	Teaching Methods	Evaluation Methods	References
1	1	**Chapter 1: The Schrodinger Equation**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 1
	2		Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 1
2	3	**Chapter 2: The Particle in a Box**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 2
	4	**Chapter 3: Operators**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 3
3	5		Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 3
	6	**Chapter 4: The Harmonic Oscillator**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 4
4	7		Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 4
	8	**Chapter 5: Angular Momentum**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 5
5	9		Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 5
	10	**Chapter 6: The Hydrogen Atom**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 6
6	11		Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 6
	12		Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 6
7	13	**Chapter 7: Theorems of Quantum Mechanics**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 7
	14		Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 7
8	15	**Chapter 8: The Variation Method**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 8
	16		Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 8

9	17	**Chapter 9: Perturbation Theory**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 9
	18		Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 9
10	19	**Chapter 10: Electron Spin**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 10
	20	**Chapter 11: Many-Electron Atoms**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 11
11	21	**Chapter 12: Computational Chemistry**	Self Reading & skills learning	Projects	Practical Comput. Chem., Helal.
	22		Self Reading & skills learning	Projects	Practical Comput. Chem., Helal.
12	23		Self Reading & skills learning	Projects	Practical Comput. Chem., Helal.
	24		Self Reading & skills learning	Projects	Practical Comput. Chem., Helal.
13	25		Self Reading & skills learning	Projects	Practical Comput. Chem., Helal.
	26		Self Reading & skills learning	Projects	Practical Comput. Chem., Helal.
14	27		Self Reading & skills learning	Projects	Practical Comput. Chem., Helal.
	28		Self Reading & skills learning	Projects	Practical Comput. Chem., Helal.

22 Evaluation Methods:

Opportunities to demonstrate achievement of the CLOs are provided through the following assessment methods and requirements:

Evaluation Activity	Mark	Topic(s)	CLO	Period (Week)	Platform
Midterm Exam	30	Chapters 1-7	CLO-1	9th Week	Written exam
Project 1	10	Computational Chemistry techniques	CLO-3	11rd Week	
Project 2	10	Computational Chemistry techniques	CLO-3	13th Week	
Project 3	10	Computational Chemistry techniques	CLO-3	15th Week	
Final Exam	40	Chapters 1-11 + Computational Chemistry techniques	CLO-1 + CLO-2 + CLO-3	16th Week	Written exam

23 Course Requirements

N/A

24 Course Policies:

A- Attendance policies:

Students should attend at least 85% of the total number of the lectures.

B- Absences from exams and submitting assignments on time:

Students who miss an exam must submit and acceptable excuse and then a makeup exam will be appointed.

C- Health and safety procedures:

Followed according to university regulations.

D- Honesty policy regarding cheating, plagiarism, misbehavior:

Followed according to university regulations.

E- Grading policy:

1. Mid exam 30%
2. Projects 30%
3. Final exam: 40%

The letter grade scale is adopted.

F- Available university services that support achievement in the course:
Central library, personal computer labs at different locations in the university, e-learning site, faculty member's website.

25 References:

A- Required book(s), assigned reading and audio-visuals:

1. I. N. Levine, ***Quantum Chemistry***, 7th ed., Pearson Education, Inc., 2014.

2. Wissam Helal, Practical Computational Chemistry, A Training Manual of Selected Short Experiments Using Gaussian & ORCA, The University of Jordan, 2023.

B- Recommended books, materials, and media:

1. P. W. Atkins, R. S. Friedman, ***Molecular Quantum Mechanics***, 5th ed., OUP, 2011.
2. J. Lowe, K. Peterson, ***Quantum Chemistry***, 3rd ed., Elsevier AP, 2006.
3. D. A. McQuarrie, ***Quantum Chemistry***, 2nd ed., University Science Books, 2007.
4. F. Pilar, ***Elementary Quantum Chemistry***, 2nd ed., McGraw-Hill, 1990.
5. J. Simons, A. Nichols, ***Quantum Mechanics in Chemistry***, OUP, 1997.

26 Additional information:

N/A

Name of Course Coordinator: Dr Wissam Helal	Signature: Wissam Helal	Date: 15/10/2023
Head of Curriculum Committee/Department: ----------	Signature: ----------	
Head of Department: ----------	Signature:----------	
Head of Curriculum Committee/Faculty: ----------	Signature: ----------	
Dean: ----------	Signature: ----------	