Course Syllabus

1	**Course title**	Applications in Quantum Chemistry
2	**Course number**	0333941
3	**Credit hours**	3 Hours
	Contact hours (theory, practical)	(3,0)
4	**Prerequisites / corequisites**	0333741
5	**Program title**	Doctor of Philosophy (PhD) in Chemistry
6	**Program code**	0303
7	**Awarding institution**	The University of Jordan
8	**School**	Science
9	**Department**	Chemistry
10	**Course level**	Postgraduate/PhD
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**	February 25-2024

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:

Applications in Quantum chemistry is the second course of the two-semester quantum chemistry sequence offered by the department of chemistry intended for post-graduates majoring in chemistry. In this course we explore advanced concepts and ideas in quantum chemistry, computational chemistry, and electronic structure theory. The course covers approximation methods (variational and perturbation theories); electronic structure of atoms and molecules; Hartree-Fock theory (HF); ab-initio methods; density functional theory (DFT); semi-empirical methods; and different computational techniques for the calculations of real chemical systems.

20 Course aims and outcomes:

A- Aims:

1. Develop a solid understanding of the fundamental principles of computational chemistry.\

2. Acquire a quantitative understanding of quantum and computational chemistry. Furthermore, students will be able to derive all relevant important mathematical and theoretical models.

4. Promote problem-solving skills by applying different mathematical and numerical methods and techniques to the solution of relevant, but relatively complex and real chemical problems.

5. Appreciate the continuous interplay between experiment and theory in computational 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 molecular structure and computational modeling.
CLO-2. Apply problem solving skills to solve chemical problems using computational 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 Variation Method**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 8
	2		Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 8
2	3	**Chapter 2: Perturbation Theory**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 9
	4		Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 9
3	5	**Chapter 3: Electron Spin**	Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 10
	6		Face to face lectures	Written Exams	Quantum. Chem., Levine, Ch 10
4	7	**Chapter 4: The Hartree-Fock Method & Basis Sets**	Face to face lectures	Written Exams	Diff Refs (see Section 25)
	8		Face to face lectures	Written Exams	Diff Refs (see Section 25)
5	9		Face to face lectures	Written Exams	Diff Refs (see Section 25)
	10		Face to face lectures	Written Exams	Diff Refs (see Section 25)
6	11	**Chapter 5: *Ab-Initio* Electron Correlation Methods**	Face to face lectures	Written Exams	Diff Refs (see Section 25)
	12		Face to face lectures	Written Exams	Diff Refs (see Section 25)
7	13		Face to face lectures	Written Exams	Diff Refs (see Section 25)
	14		Face to face lectures	Written Exams	Diff Refs (see Section 25)

8	15	**Chapter 6: Semi-Empirical Quantum Chemistry Methods**	Face to face lectures	Written Exams	Diff Refs (see Section 25)
	16	**Chapter 7: Semi-Empirical Quantum Chemistry Methods**	Face to face lectures	Written Exams	Diff Refs (see Section 25)
9	17		Face to face lectures	Written Exams	Diff Refs (see Section 25)
	18		Face to face lectures	Written Exams	Diff Refs (see Section 25)
10	19	**Chapter 8: Computational Chemistry**	Self Reading & skills learning	Projects	Practical Comput. Chem., Helal.
	20		Self Reading & skills learning	Projects	Practical Comput. Chem., Helal.
11	21		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. P. W. Atkins, R. S. Friedman, ***Molecular Quantum Mechanics***, 5th ed., OUP, 2011.

3. J. Lowe, K. Peterson, ***Quantum Chemistry***, 3rd ed., Elsevier AP, 2006.

4. D. A. McQuarrie, ***Quantum Chemistry***, 2nd ed., University Science Books, 2007.

5. A. Szabo, N. Ostlund, ***Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory,*** 1st ed. revised, McGraw-Hill, 1989.

6. T. Helgaker, P. Jorgensen, J. Olsen, ***Molecular Electronic-Structure Theory,*** Wiley, 2000.

7. C. J. Cramer, ***Essentials of Computational Chemistry, Theories and Models,*** 2nd ed., Wiley, 2004.

8. F. Jensen, ***Introduction to Computational Chemistry,*** 3rd ed., John Wiley, 2017.

9. 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:

Recent research articles and reviews will be assigned and recommended for different topics covered during the course.

26 Additional information:

N/A

Name of Course Coordinator: Dr Wissam Helal	Signature: Wissam Helal	Date: 25/3/2024
Head of Curriculum Committee/Department: ----------	Signature: ----------	
Head of Department: ----------	Signature:----------	
Head of Curriculum Committee/Faculty: ----------	Signature: ----------	
Dean: ----------	Signature: ----------	