Form: Course Syllabus	Form Number	EXC-01-02-02A
	Issue Number and Date	2/3/24/2022/2963 05/12/2022
	Number and Date of Revision or Modification	
	Deans Council Approval Decision Number	2/3/24/2023
	The Date of the Deans Council Approval Decision	23/01/2023
	Number of Pages	06

1.	**Course Title**	Applications in Quantum Chemistry
2.	**Course Number**	0333941
3.	**Credit Hours (Theory, Practical)**	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.	**School/ Center**	Science
8.	**Department**	Chemistry
9.	**Course Level**	Postgraduate/PhD
10.	**Year of Study and Semester (s)**	First or second year, Fall or Spring semesters
11.	**Other Department(s) Involved in Teaching the Course**	N/A
12.	**Main Learning Language**	English
13.	**Learning Types**	☒ Face to face learning ☐ Blended ☐ Fully online
14.	**Online Platforms(s)**	☐ Moodle ☒ Microsoft Teams
15.	**Issuing Date**	February 20, 2024
16.	**Revision Date**	November 24, 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:

Name:
Office number:
Phone number:
Email:
Contact hours:
Name:
Office number:
Phone number:
Email:
Contact hours:

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. Program Student Outcomes (SO's): (To be used in designing the matrix linking the intended learning outcomes of the course with the intended learning outcomes of the program)

SO1. Develop chemistry expertise, focus on theory and practice, and contribute to advancing knowledge in a specific research field.

SO2. Conduct original, high-quality research that advances knowledge in chemistry by developing complex projects using innovative methodologies.

SO3. Mentor junior researchers and students and demonstrate leadership in the scientific community through collaboration, peer review, and knowledge exchange.

SO4. Recognize the ethical implications and responsibly use chemistry solutions to tackle global challenges.

SO5. Participate in ongoing professional development to stay up to date with the latest research and innovations.

21. Course Intended Learning Outcomes (CLO's): (Upon completion of the course, the student will be able to achieve the following intended learning outcomes)

1. Acquire fundamental conceptual way of thinking related molecular structure and computational modeling.

2. Apply problem solving skills to solve chemical problems using computational chemistry methods.

3. Gain working experience with different computational chemistry tools.

Course CLOs	The learning levels to be achieved					
	Remembering	**Understanding**	**Applying**	**Analysing**	**evaluating**	**Creating**
1		**X**		**X**		
2		**X**		**X**		
3			**X**	**X**		

22. The matrix linking the intended learning outcomes of the course with the intended learning outcomes of the program:

Program SO's / Course CLO's	SO (1)	SO (2)	SO (3)	SO (4)	SO (5)
CLO (1)	X	X			
CLO (2)	X	X			
CLO (3)	X	X			

23. Topic Outline and Schedule:

Week	Lecture	Topic	CLO/s Linked to the Topic	Learning Types Face to Face (FF) Blended (BL) Fully Online (FO)	Platform Used	Synchronous (S) Asynchronous (A)	Evaluation Methods	Learning Resources
1	1.1	**Chapter 1: The Hartree-Fock Method & Basis Sets**	1,2	FF			Written Exams	Diff Refs (See sec 25)
	1.2		1,2	FF				
2	2.1		1,2	FF			Written Exams	Diff Refs (See sec 25)
	2.2		1,2	FF			Written Exams	Diff Refs (See sec 25)
3	3.1		1,2	FF				
	3.2	**Chapter 2: *Ab-Initio* Electron Correlation Methods**	1,2	FF			Written Exams	Diff Refs (See sec 25)
4	4.1		1,2	FF				
	4.2		1,2	FF			Written Exams	Diff Refs (See sec 25)
5	5.1		1,2	FF				
	5.2		1,2	FF			Written Exams	Diff Refs (See sec 25)
6	6.1		1,2	FF				
	6.2		1,2	FF				
7	7.1	**Chapter 3: Semi-Empirical Quantum Chemistry Methods**	1,2	FF			Written Exams	Diff Refs (See sec 25)
	7.2		1,2	FF				
8	8.1		1,2	FF			Written Exams	Diff Refs (See sec 25)
	8.2		1,2	FF				
9	9.1		1,2	FF			Written Exams	Diff Refs (See sec 25)
	9.2		1,2	FF				

10	10.1	**Chapter 4: Density Functional Theory**	1,2	FF			Written Exams	Diff Refs (See sec 25)
	10.2		1,2	FF				
11	11.1		1,2	FF			Written Exams	Diff Refs (See sec 25)
	11.2		1,2	FF				
12	12.1	**Chapter 12: Computational Chemistry**	2,3	FF			Projects	Practic. Comput Chem., Helal.
	12.2		2,3	FF			Projects	Practic. Comput Chem., Helal.
13	13.1		2,3	FF			Projects	Practic. Comput Chem., Helal.
	13.2		2,3	FF			Projects	Practic. Comput Chem., Helal.
14	14.1		2,3	FF			Projects	Practic. Comput Chem., Helal.
	14.2		2,3	FF			Projects	Practic. Comput Chem., Helal.
15	15.1		2,3	FF			Projects	Practic. Comput Chem., Helal.
	15.2		2,3	FF			Projects	Practic. Comput Chem., Helal.
16							Final Exam	

24. Evaluation Methods:

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

Evaluation Activity	Mark	Topic(s)	CLO/s Linked to the Evaluation activity	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

25. Course Requirements:

Students should have a personal computer or at least an access to a PC. Appropriate software and program codes will be provided.

26. Course Policies:

A- Attendance policies:

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

1. 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.

2. Health and safety procedures:
   Followed according to university regulations.

3. Honesty policy regarding cheating, plagiarism, misbehavior:
   Followed according to university regulations.

4. 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.

27. 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.

28. Additional information:

NA

Name of the Instructor or the Course Coordinator: Dr. Wissam Helal	Signature: Wissam Helal	Date: November 24, 2024
The Head of Graduate Studies Committee/ Department Chemistry **Dr. Murad AlDamen, Prof.**	**Signature:** **……...……**	**Date:** **……..……**
The Head of Department of Chemistry **Dr. Murad AlDamen, Prof.**	**Signature:** **……...……**	**Date:** **……..……**
Vice Dean for Graduate Studies and Scientific Research / School of Science **Dr. Kamal Sweidan, Prof.**	**Signature:** **……...……**	**Date:** **……..……**
The Dean of School of Science **Dr. Mahmoud I. Jaghoub, Prof.**	**Signature:** **……...……**	**Date:** **……..……**