Course Syllabus

1	**Course title**	Software Packages in Chemistry
2	**Course number**	0303361
3	**Credit hours**	2 Hours
	Contact hours (theory, practical)	(1,3)
4	**Prerequisites / corequisites**	0303341
5	**Program title**	Bachelor degree in chemistry
6	**Program code**	0303
7	**Awarding institution**	The University of Jordan
8	**School**	Science
9	**Department**	Chemistry
10	**Course level**	3rd year
11	**Year of study and semester (s)**	Fall, Spring and Summer
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**	July 1-2024

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:

Software Packages in Chemistry course offers the opportunity for chemistry majors to perform experiments related to some of the main software used by the chemical scientific community. The experiments covers three main types of utilities: Spreadsheets, chemical drawing software, and computational chemistry software.

20 Course aims and outcomes:

A- Aims:

1. Develop a firm and solid understanding of the fundamental principles of physical chemistry.
2. Explain the fundamental concepts and phenomena of physical chemistry, in particular, in electrochemistry and electrochemical equilibrium, chemical kinetics and reaction dynamics, reaction mechanisms, catalysis, and surface chemistry.
3. Acquire a quantitative understanding of physical chemistry, by both expressing ideas and 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 problems, and by encouraging students to work systematically through complex problems.
5. Appreciate the continuous interplay between experiment and theory in physical chemistry.
6. Allow students to develop an awareness of the connections between topics in physical chemistry, in order to explore physical chemistry as a "unified" field of study and research.
7. Integrate the fundamental subjects learned with practical and industrial applications.
8. Stimulate student's interest to the state of art techniques and developments in the field of physical chemistry, through chemical primary sources and literature.

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

CLO-1. Acquire numerical skills for the analysis of chemical data.
CLO-2. Apply problem solving skills to solve chemical problems using automated and numerical tools.
CLO-3. Acquire working experience with different computational chemistry tools.

0303361 Software Packages in Chemistry								
		Student Outcomes (SO)						
		SO-1	SO-2	SO-3	SO-4	SO-5	SO-6	SO-7
Course Learning Outcomes (CLO)	CLO-1	✓		✓				
	CLO-2	✓		✓				
	CLO-3	✓		✓				

21. Topic Outline and Schedule:

Week	Lecture/Experiment	Topic	Teaching Methods/platform	Evaluation Methods	References
2	1	**Experiment 1:** Excel: Basic operations and functions	Practical in the computer laboratory	Reports + Mid and Final exams	Software Packages in Chem Experiment 1
3	2	**Experiment 2:** Excel: Graphs and plots	Practical the computer laboratory	Reports + Mid and Final exams	Software Packages in Chem Experiment 2
4	3	**Experiment 3:** Mathematical Methods in Excel	Practical in the computer laboratory	Reports + Mid and Final exams	Software Packages in Chem Experiment 3
5	4	**Experiment 4:** Excel: Curve fitting and linear regression	Practical in the computer laboratory	Reports + Mid and Final exams	Software Packages in Chem Experiment 4
6	5	**Experiment 5:** Chemsketch: Drawing basic and complex structural formulas	Practical in the computer laboratory	Reports + Mid and Final exams	Software Packages in Chem Experiment 5
7	6	**Experiment 6:** Chemsketch: Drawing chemical reactions and schemes	Practical in the computer laboratory	Reports + Mid and Final exams	Software Packages in Chem Experiment 6
8	7	**Experiment 7:** Gaussian: Basic calculations	Practical in the computer laboratory	Reports + Final exam	Software Packages in Chem Experiment 7
9	8	**Experiment 8:** Gaussian: Molecular orbitals, electron density and electrostatic potentials	Practical in the computer laboratory	Reports + Final exam	Software Packages in Chem Experiment 8
10	9	**Experiment 9:** Gaussian: Geometry Optimization and Vibrational Frequencies	Practical in the computer laboratory	Reports + Final exam	Software Packages in Chem Experiment 9
11	10	**Experiment 10:** Gaussian: Including Solvent & Solvation	Practical in the computer laboratory	Reports + Final exam	Software Packages in Chem Experiment 10
12	11	**Experiment 11:** Locating & Optimizing Transition States	Practical in the computer laboratory	Reports + Final exam	Software Packages in Chem Experiment 11
13	12	**Experiment 12:** Reaction Coordinate Scans & Potential Energy Surfaces	Practical in the computer laboratory	Reports + Final exam	Software Packages in Chem Experiment 12

22 Evaluation Methods:

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

Evaluation Activity	Mark	Topic(s)	CLO	Period (Week)	Platform
Reports	40	All Experiments		All weeks	Written
Mid exam	20	Experiments 1-6		Week 8	Written exam
Final exam	40	Experiments 1-10		Final exams 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 20%
2. Reports 40%
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 readings and audio-visuals:
Wissam Helal, Software Packages in Chemistry: A Manual of Selected Experiments Using Excel, Chemsketch & Gaussian, The University of Jordan 2023.

B- Recommended books, other materials, and media:
Lecture notes and other documents and information relevant to the course are available at my e- leering site of The University of Jordan (https://elearning.ju.edu.jo//).

Furthermore, students are strongly recommended to frequently consult one or more of the following books (all available at the university library):

1. P. W. Atkins, and J. de Paula, Atkins' Physical Chemistry, 10th ed., OUP, 2014.
2. G. Barrow, Physical Chemistry, 6th ed., McGraw-Hill College, 1996.
3. T. Engel, and P. Reid, Physical Chemistry, 3rd ed., Pearson Education, Inc., 2013.
4. I. N Levine, Physical Chemistry, 6th ed., the McGraw-Hill Companies, 2009.
5. R. Silbey, R. Alberty, and M. Bawendi, Physical Chemistry, 4th ed., John Wiley, 2004.

26 Additional information:

N/A

Name of Course Coordinator: Dr Wissam Helal Signature: Wissam Helal Date: 1/7/2024
Head of Curriculum Committee/Department: ---------- Signature: ----------
Head of Department: ---------- Signature:----------
Head of Curriculum Committee/Faculty: ---------- Signature: ----------
Dean: ---------- Signature: ----------