Department of Chemistry

College of Education

Salahaddin University-erbil

Subject: Quantum Chemistry

Course Book – Stage four

Lecturer's name Prof. Dr. Hassan H. Abdallah

Academic Year: 2023/2024

Course Book

1. Course name	**Quantum Chemistry**
2. Lecturer in charge	**Prof. Dr. Hassan H. Abdallah**
3. Department/ College	**Chemistry Dep. College of Education**
4. Contact	**e-mail: Hassan.abdullah@su.edu.krd** **Tel: (optional)**
5. Time (in hours) per week	**Theory: 2**
6. Office hours	**Monday 9.30 am - 11.30 am** **Tuesday 10.30 am - 12.30 pm** **Wednesday 8.30 am – 11.30 am** **or by appointment**
7. Course code	
8. Teacher's academic profile	**https://scholar.google.com/citations?user=hassan=en**
9. Keywords	**Quantum mechanics, Schrödinger equation, Approximation methods, SCF methods**

10. Course overview:

Quantum Chemistry shows the background and the principles of all branches of Chemistry, namely, inorganic, organic, spectroscopy and physical chemistry. This course presents an introduction to quantum mechanics. It begins with an examination of the historical development of quantum theory, properties of particles and waves, wave mechanics and applications to simple systems, including the particle in a box, the harmonic oscillator, the rigid rotor and the hydrogen atom. The lectures continue with a discussion of atomic structure. The final lectures cover applications to chemical bonding including Hückel theory, molecular orbital theory and modern electronic structure theories. Graduate students with understanding of quantum chemistry will enable them to be successful candidates for postgraduate studies and to work in research centers and pharmaceutical companies and as a teacher in schools and universities.

11. Course objective:

The objectives of this course involve the explanation of the beginning and historical development of the quantum mechanics, to calculate different physical properties using the operator, eigen function and eigen value, to apply the techniques of quantum mechanics to solve the Schrödinger equation for one and many-electrons systems, to explain and apply the approximation methods to solve the Schrodinger equation for the atomic and molecular systems, to introduce the basic molecular orbital theories as well as briefly describing the various modern theories and to calculate chemical and physical properties theoretically using different quantum mechanics methods.

12. Student's obligation

The students should attend all the lectures, should pass the final exam and do all the tests and quizzes, should participate in discussion and question and answer activity.

13. Forms of teaching

Lectures (power point and hand out); Tutorials; Discussions; Independent study; Individual assignments

14. Assessment scheme

The students are required to do at least two tests during the course and a number of quizzes and home work.

15. Student learning outcome:

- ✓ Explain the historical development and the principles of quantum mechanics.
- ✓ Apply the techniques of quantum mechanics to solve the Schrödinger equation for one and many-electrons systems.
- ✓ Explain and apply the approximation methods to solve the Schrodinger equation for the atomic and molecular systems.
- ✓ Introduce the basic molecular orbital theories as well as briefly describing the various modern theories.
- ✓ Calculate chemical and physical properties theoretically using different quantum mechanics methods.
- ✓ Studying the spectroscopic results of organic and inorganic compounds.

16. Course Reading List and References:

1. McQuarrie, Donald A. Quantum Chemistry. 2nd ed. Sausalito, CA: University Science Books, 2007.
2. P. W. Atkins. Physical Chemistry 8th ed. Oxford University Press. 2006.
3. P. W. Atkins, R. S. Friedman, Molecular Quantum Mechanics, Oxford University Press, 2005.
4. I. N. Levine, Quantum Chemistry, Prentice-Hall, Upper Saddle River. 2000.
5. L. Pauling, E. B. Wilson, Introduction to Quantum Mechanics with Applications to Chemistry. Dover. New York. 1985.
6. L. Pauling. The Nature of Chemical Bonds. Cornell University Press. Ithaca. 1960.
7. Internet.

17. The Topics:	Lecturer's name
Week 1, Introduction of quantum mechanics, Discovery of the electron and structure of the atom.	Dr. Hassan H. Abdallah Each lecture is 2 hrs

Week 2, Blackbody radiation and photoelectric effect, The atom of Niels Bohr, Wave-particle duality of light and matter, Uncertainty principle. **Week 3,** Principles of quantum mechanics, operator, eigen function and eigen value. **Week 4,** The postulates of quantum mechanics I. **Week 5,** The postulates of quantum mechanics II. **Week 6,** Particle in a box, one and multi dimensions, Applications of the system of particle in a box. **Week 7,** Quantum mechanical harmonic oscillator. **Week 8,** Rigid rotator. **Week 9,** Hydrogen atom. **Week 10,** Applications and comparisons. **Week 11,** Many electron atoms, Approximation methods. **Week 12,** Variation theory and Perturbation theory. **Week 13,** Hartree method. **Week 14,** Slater determinant, Hartree-Fock method. **Week 15,** Systems of many-electron molecules. **Week 16,** Hückel theory. **Week 17,** Applications of Hückel theory. **Week 18,** Molecular orbital theory. **Week 19,** Study week.	
18. Practical Topics (If there is any)	
No practical topics	

19. Examinations:

1. Compositional: In this type of exam the questions usually starts with Explain how, What are the reasons for…?, Why…?, How….?

Examples:

- Explain the applications of Schrödinger equation.
- Compare between Hartree and Hartree-Fock methods.

2. True or false type of exams:

In this type of exam a short sentence about a specific subject will be provided, and then students will comment on the trueness or falseness of this particular sentence.

Examples:

- The calculated total electronic energy for a system is the same according to Hartree and Hartree-Fock methods, true or false?
- The electron has particle properties only, true or false?

3. Multiple choices:

In this type of exam there will be a number of phrases next or below a statement, students will match the correct phrase.

20. Extra notes:

21. Peer review