Theoretical Chemistry

1. **Course number and name:** 020CHTCS1 Theoretical Chemistry

2. **Credits and contact hours:** 4 ECTS credits, 2x1:15 contact hours

3. **Names of instructors:** Roger LTEIF

4. **Instructional materials:**
   - Course handouts
   - References
     - Catalyse de contact (conception, préparations et mise en œuvre des catalyseurs industriels) J.F. Le Page et coll. (TECNIP, 1978)
     - Chimie physique générale ; atomistique, liaisons chimiques et structures moléculaires G. Pannetier (Masson, 1962)
     - Elements de chimie quantique à l'usage des chimistes Jean-Louis Rivail (EDP Sciences, CNRS éditions, 1999)
     - Physical chemistry P. W. Atkins (Oxford University Press, 1990)
     - Chimie quantique, de l'atome à la théorie de Hückel Bernard Vidal (Masson, 1992)
     - Exercices de Chimie quantique Bernard Vidal (Masson, 1995)
     - Quantum chemistry H. Eyring, J. Walter, G.E. Kimball (J. Wiley, NewYork 1958)
     - Modern quantum chemistry Szabo, N.S. Ostlund (Macmillan, NewYork 1982)
     - Elementary quantum chemistry Frank L. Pilar (McGraw-Hill, 1990)
     - Chimie quantique. Exercices et problèmes résolus Claude Millot et Xavier Assfeld (Dunod, 2000)
     - Quantum chemistry Ira N. Levine (Prentice-Hall, Inc. 1991)
     - Mécanique Quantique C. Cohen-Tannoudji, B. Diu, F. Laloë
     - Orbitales frontières : manuel pratique (InterEditions /CNRS Editions, 1995) N. Trong Anh
     - Manuel de chimie théorique : Application a la structure et à la réactivité en chimie moléculaire (Ellipses, 2000) Patrick Chaquin

5. **Specific course information**
   a. **Catalog description:**
      This course provides:
      - An introduction to quantum phenomena, the postulates of Quantum mechanics: angular momentum, the hydrogen atom.
      - The major approximation methods: variational principle, perturbation theory.
      - The polyelectronic atoms: the atomic orbital approximation.
      - Molecular orbital approximation and quantum chemical methods: Hartree-Fock, Hückel method. Application to diatomic and polyatomic molecules; role of spatial symmetry. Introduction to responsiveness. Approximation of frontier orbitals.
      - Spectra of vibration, rotation and electronic transition of molecules: Study the spectra of vibration, rotation and electronic transition.

b. Prerequisites: 020ATONI2 Atomic Structure and chemical Bonding

c. Required/Selected Elective/Open Elective: Required

6. Specific goals for the course

a. Specific outcomes of instruction:

- Explain the nature and behavior of electromagnetic radiation using the wave model.
- Explain the photoelectric effect using the quantum model.
- Conceptualize the atomic model of quantum mechanics.
- Understand and master the essential concepts of quantum mechanics used in chemistry.
- Solve the Schrödinger equation for simple chemical systems (hydrogenoid atoms, polyelectronic atoms)
- Explain the effect of a magnetic field on the energy levels of an atom.
- Understand the quantum origin of chemical concepts (chemical bond and hybrid atomic orbitals, aromaticity, conjugated systems π in Hückel's method) and make the link with the quantities that can be measured experimentally (bond lengths, wavelengths of absorption, ionization energies, ...)
- Explain the rotation, vibration and electronic transition spectra of diatomic and polyatomic molecules

b. PIs addressed by the course:

PI	1.1	1.2	1.3
Covered	x	x	x
Assessed	x	x	x

7. Brief list of topics to be covered

- Chapter I- General introduction to quantum mechanics:
  Origins of quantum mechanics, the principles of quantum mechanics, the dynamics of atomic and molecular (microscopic) systems and the postulates of quantum mechanics in the case of a particle in a box.
  Exercises Series 1

- Chapter II- Single-electron atom; hydrogen or hydrogenoid:
  Study the hydrogen atom and hydrogenoids as well as the radial and angular equations and the interpretation of the wave functions of hydrogenoids.
  Exercises Series 2

- Chapter III- Polyelectronic atoms:
  Study the case of He atom and the polyelectronic atoms: from the independent model to an approximate method.
  Exercises Series 3

- Chapter IV- Influence of a magnetic field on energy levels: Study the energy diagrams in the presence of a magnetic field, the normal and anomalous Zeeman effect.
  Exercises Series 4

- Chapter V- Chemical bonds and molecular orbitals: Study the H_2^+ chemical bond and the LCAO approximation, diatomic molecules, unsaturated molecules, the principles of Hückel's method and simple molecules.
  Exercises Series 5

- Chapter VI- Optical methods for studying molecules: Studying the vibration, rotation and electronic transition spectra of molecules in the case of diatomic and polyatomic molecules. Explain the Frank-Condon principle and the Jablonski-Perrin diagram. Exercises Series 6