UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

# COURSE SYLLABUS

# Chimica Fisica Superiore - Modulo 1

**2122-1-F5401Q027-M1**

## Aims

To provide students with the fundamentals of quantum chemistry and present the main methods for calculating structure and properties of molecular systems.

**Knowledge and understanding**

- The main postulates and theorems of quantum chemistry.
- Methods for calculating properties of atomic and molecular systems.
- The appropriate formalism to treat quantum chemical problems.

**Applying knowledge and understanding**

Methodologies and mathematical instruments useful to solve the Schrödinger equation for many-electron systems.

**Making judgements**

- Evaluation of potentialities and limitations of the different methodologies.
- Ability in selecting the most appropriate method to calculate diverse properties for systems with different complexity.

**Communication skills**

Rigorous use of scientific language and of the quantum chemistry formalism.

**Learning skills**
Activation of critical skills in the analysis of scientific models.

## Contents

Principles of quantum mechanics. Variation method and perturbation theory. Many-electron atoms. Molecular electronic structure.

## Detailed program

- Review of the main principles of quantum mechanics.
- Solutions to the Schrödinger equation for many-electron systems: the variation method and the perturbation theory.
- Electron spin and antisimmetry.
- Many-electron atoms.
- Molecular electronic structure: the Born-Oppenheimer approximation; the Molecular Orbital theory. The Hartree-Fock method for MO-LCAO calculations. Example calculations of molecular electronic structures.

## Prerequisites

Basic knowledge of mathematics, physics and quantum chemistry.

## Teaching form

Lessons.

## Textbook and teaching resource

Textbook: I.N. Levine, Quantum Chemistry, Prentice Hall; slides from the docent

## Semester

First semester

## Assessment method

Oral examination. The exam aims at verifying the level of knowledge acquired, the understanding of conceptual approach in the development of the theory presented during the class and the appropriate use of the language by the student.

The final mark of the course "Advanced Physical Chemistry" is the average of the evaluations obtained in the 2 modules. The students can undergo the exams of the 2 modules separately.

## Office hours

By appointment