

COURSE: PHYSICAL CHEMISTRY II

ACADEMIC YEAR: **2018-2019**

TYPE OF EDUCATIONAL ACTIVITY: Characterizing

TEACHER: **Camilla Minichino**e-mail: **camilla.minichino@unibas.it**website: <http://scienze.unibas.it/site/home.html>phone: **0971-206158**

mobile (optional):

Language: ITALIAN

ECTS: (lessons e
tutorials/practice) **6**n. of hours: (lessons e
tutorials/practice) **48**Campus: Potenza
Dept./School: **Dipartimento di
Scienze**
Program: : **CHIMICA(L27)**Semester: **II**
From 01 march untill
31 may-30 june 2019**EDUCATIONAL GOALS AND EXPECTED LEARNING OUTCOMES**

The aim of the course is to provide a basic understanding of the principles and techniques of quantum mechanics in order to refine the skills in the theoretical description of the structure and properties of atoms and molecules. At the end of the course the students must demonstrate to a) know the fundamentals of quantum mechanics and the models that form the basis of the theory of chemical bonding and molecular spectroscopy; b) comprehend the formal and logical path for characterizing the electronic states of atoms and molecules; c) be able to solve qualitative and simple quantitative problems in quantum mechanics applied to chemistry.

PRE-REQUIREMENTS

General chemistry, differential and integral calculus, linear algebra, classical mechanics, electromagnetism and waves.

SYLLABUS**Fundamentals and simple applications of quantum mechanics**

Origins of the quantum theory. Postulates and some fundamental principles of quantum mechanics in the coordinate representation of Schrödinger. The time-independent Schrödinger equation in piecewise constant potentials and its applications in chemistry. The harmonic oscillator and the molecular vibrations. The orbital angular momentum and the spectroscopic model of the rigid rotor. Hydrogen-like atoms. Overview of Dirac formulation of quantum mechanics. Variational method and time-independent perturbation theory. Generalized angular momentum, spin, the angular momentum in composite systems, magnetic moments and spin-orbit coupling, fine and hyperfine structure of one-electron atom. Identical particles and symmetrization/antisymmetrization postulate.

Atomic Structure

Polyelectronic atoms: separability and orbital approximation, Slater determinant as antisymmetric wavefunction of independent electrons, self-consistent construction of the effective potential, electronic configuration, coupling schemes of angular momenta and electronic states.

Molecular Structure

Molecular symmetry and group theory. Introduction to the molecular structure: separation between nuclear and electronic motions, definition and characterization of the potential energy surface, The solution of electronic problem: fundamentals of molecular orbital and valence bond theories. Classification and qualitative building of molecular orbitals, the Hückel method, electronic configurations, electronic states and molecular term symbols.

TEACHING METHODS

Theoretical lessons.

EVALUATION METHODS

Oral examination.

TEXTBOOKS AND ON-LINE EDUCATIONAL MATERIAL

- Lecture notes and presentations slides (<https://cloud.unibas.it/index.php/s/OXiqrCnITYUouC>)
- *Textbook*
P. W. Atkins e R. Friedman. *Meccanica Quantistica Molecolare*, Zanichelli (2000).

○ *Additional Readings*

C. Cohen-Tannoudji, B. Diu, and F. Laloe. *Quantum Mechanics. Vol. 1 e 2*, Wiley (1977).

R.P. Feynman, R.P.; R.B. Leighton, e M. Sands. *La fisica di Feynman. Vol3: Meccanica Quantistica*, Zanichelli (2007).

L. Piela. *Ideas of Quantum Chemistry*, II Edition, Elsevier (2013).

A. Balzarotti, M. Cini e M. Fanfoni. *Atomi, Molecole e Solidi, Esercizi Risolti*, Seconda Edizione, Springer (2018).

INTERACTION WITH STUDENTS

At the beginning of the course the instructor, after describing goals, learning objectives, detailed course topics, evaluation method, provides educational material on cd or pendrive and gives the password for accessing the link (<https://cloud.unibas.it/index.php/s/OXiqrCnITYUouC>) where the (eventually updated) material is stored. The lecturer also collects a list of students together with name, family name, e-mail and possibly cell phone number and reminds to be always available for providing help and assistance.

Office hours: usually on Monday and Wednesday 11:00am-1:00 pm in 3D-103B room (please send an e-mail in advance) or in different hours/days by appointment.

EXAMINATION SESSIONS (FORECAST)¹

21/01/2019, 18/02/2019, 11/03/2019, 15/04/2019, 20/05/2019, 10/06/2019, 01/07/2019, 22/07/2019, 09/09/2019, 07/10/2019, 16/12/2019.

SEMINARS BY EXTERNAL EXPERTS YES NO

FURTHER INFORMATION

Attendance: not required, but strongly recommended.

¹ Subject to possible changes: check the web site of the Teacher or the Department/School for updates.