DIPARTIMENTO DI SCIENZE

COURSE: **PHYSICAL CHEMISTRY II**	
ACADEMIC YEAR: **2019-2020**	
TYPE OF EDUCATIONAL ACTIVITY: Characterizing	
TEACHER: **Camilla Minichino**	
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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 02.03.2020 to 31.05- 20.06 2020**

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:

- master the elementary principles and methods of quantum mechanics,
- know the keys models in the theory of chemical bond and molecular spectroscopy,
- understand the formal and conceptual pathway to characterize the electronic states of atoms and molecules,
- be able to solve simple quantum mechanical problems applied to chemistry in a qualitative and quantitative way
- know how to interpret experimental observables in terms of molecular properties,
- link the formal tools of molecular quantum mechanics with the concepts acquired in previous courses,
- be able to systematically organize the acquired knowledge and express it using the correct terminology.

PRE-REQUIREMENTS

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

SYLLABUS

Fundamentals and simple applications of quantum mechanics (24h)

Origins of the quantum theory. Postulates and some fundamental principles of quantum mechanics in the coordinate representation of Schrödinger and a brief overview of Dirac formulation. The time-independent Schrödinger equation in piecewise constant potentials and its applications in chemistry. A minimal introduction to radiation-matter interaction and the meaning of transition moment. The harmonic oscillator and the molecular vibrations. The orbital angular momentum and the spectroscopic model of the rigid rotor. Hydrogen-like atoms. 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 (10 h)

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 (24 h)

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 and, optional, workshop-tutorial classes.

EVALUATION METHODS

Oral examination.

Optional periodic tests for self-assessment of acquired knowledge, comprehension, and skills.

TEXTBOOKS AND ON-LINE EDUCATIONAL MATERIAL

- Lecture notes and presentations slides (https://cloud.unibas.it/index.php/s/bQUHfxc42JARX87 e/o https://elearning.unibas.it/)
- *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, gives the password for accessing the link where the course 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 are normally on Tuesdays and Wednesdays 11 am : 1 pm in room 3D-103B (changes in the schedule may occur, due to official and institutional duties, therefore send an e-mail in advance) or in different hours/days by appointment.

EXAMINATION SESSIONS (FORECAST)[1]

21/01/2020, 04/02/2020, 20/02/2020, 03/03/2020, 26/05/2020, 09/06/2020, 07/07/2020, 21/07/2020, 15/09/2020, 06/10/2020, 15/12/2020.

SEMINARS BY EXTERNAL EXPERTS YES □ NO X

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.