DIPARTIMENTO DI SCIENZE

COURSE: PHYSICAL CHEMISTRY II			
ACADEMIC YEAR: **2016-2017**			
TYPE OF EDUCATIONAL ACTIVITY: Characterizing			
TEACHER: **Prof. Camilla Minichino**			
e-mail: **camilla.minichino@unibas.it**		website:	
phone: **0971206158**		mobile (optional): **3204371123**	
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**

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) understand the link between quantum mechanics and symmetry and be able to make use of group theory in the study of the electronic structure of 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 (24 hours)

Origins of the quantum theory. Postulates and some fundamental principles of quantum mechanics in the coordinate representation of Schrödinger. The time-independent Schrödinger equation for one- dimensional systems 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 (6 hours)

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 and electronic states.

Molecular Sructure (18 hours)

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. Overview of *ab initio*, semiempirical and DFT methods for computing the electronic structure and properties of molecules..

TEACHING METHODS

Theoretical lessons.

EVALUATION METHODS

Oral examination.

TEXTBOOKS AND ON-LINE EDUCATIONAL MATERIAL

- *On line educational material (https://cloud.unibas.it/index.php/s/g88gKe6KeOj9SQK)*
- *Textbook*

  P. W. Atkins, P.W e Friedman,R. (2000), Meccanica Quantistica Molecolare. Zanichelli..
- *Additional Readings*

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

  Feynman, R. P.; Leighton, R. B. e Sands, M. (2007), La fisica di Feynman. Vol 3:Meccanica Quantistica, Zanichelli.

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

  Rigamonti, A. and Carretta, P. (2015), Structure of Matter: An Introductory Course with Problems and Solutions: III Edition, Springer.

INTERACTION WITH STUDENTS

At the beginning of the course, after describing the objectives, program and methods of verification, the instructor provides students educational materials (https://cloud.unibas.it/index.php/s/g88gKe6KeOj9SQK) and collects a list of students who intend to enroll in the course, together with name, family name, e-mail and possibly cell phone number.

Office hours: Monday from 13 to 15 in 3D-103B room and Tuesday from 13 to 15 in 3D-103B room.

In addition the instructor is available at all times for a contact with the students through e-mail or cell phone service.

EXAMINATION SESSIONS (FORECAST)[1]

10/01/2017, 07/2/2017 , 07/03/2017, 30/05/2017, 27/06/2017, 25/07/2017, 12/09/2017, 03/10/2017, 19/12/2017.

SEMINARS BY EXTERNAL EXPERTS YES □ NO ■

FURTHER INFORMATION

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