UNIVERSITÀ DEGLI STUDI DI PALERMO

DEPARTMENT	Fisica e Chimica - Emilio Segrè
ACADEMIC YEAR	2016/2017
MASTER'S DEGREE (MSC)	CHEMISTRY
SUBJECT	THEORETICAL AND COMPUTATIONAL CHEMISTRY
TYPE OF EDUCATIONAL ACTIVITY	B
AMBIT	50483-Discipline chimiche inorganiche e chimico-fisiche
CODE	16581
SCIENTIFIC SECTOR(S)	CHIM/02
HEAD PROFESSOR(S)	FERRANTE FRANCESCO Professore Associato Univ. di PALERMO
OTHER PROFESSOR(S)	
CREDITS	6
INDIVIDUAL STUDY (Hrs)	94
COURSE ACTIVITY (Hrs)	56
PROPAEDEUTICAL SUBJECTS	
MUTUALIZATION	
YEAR	1
TERM (SEMESTER)	1° semester
ATTENDANCE	Not mandatory
EVALUATION	Out of 30
TEACHER OFFICE HOURS	**FERRANTE FRANCESCO** Tuesday 14:00 18:00 Viale delle Scienze, edificio 17, ufficio P1080 Thursday 14:00 18:00 Viale delle Scienze, edificio 17, ufficio P1080

DOCENTE: Prof. FRANCESCO FERRANTE

PREREQUISITES	Essentials of vectorial and matricial algebra; elementary quantum mechanics
LEARNING OUTCOMES	- Knowledge and comprehension of quantum mechanics and quantum chemistry - Ability to apply quantum mechanics concepts in the chemical field, particularly in the molecular electronic structure and deriving chemical and physical properties - Independent judgement in the application of models for solving the polyelectron problem in chemical applications - Communication capability of quantum chemistry concepts and problems - Ability to read academic textbooks about methods and applications of quantum chemistry, and of scientific papers reporting original researches
ASSESSMENT METHODS	One oral examination Grade in thirtieth The exam consists of not less than two questions and is thought to verify the knowledge about the course contents and the critical comprehension of the fundamental concepts. Questions begin with a very generic topic, which will be detailed thoroughly during the examination. Student should: - show adequate speaking ability - frame in the strict right context concepts such as wavefunction, atomic and molecular orbitals, molecular properties, transition between energy levels - show knowing of powers and limitations of the various approaches for the calculation of electronic structure Criteria for judgement: 30 cum laude: Beyound those criteria leading to a 30/30 grade, the student showed a real interest for the course arguments, he indipendently pondered on them and achieved a full comprehension 30: Excellent knowing of the course arguments, brilliant speaking ability, good analitic ability, excellent ability on applications. 26-29: Good knowing of the course arguments, good speaking ability, good ability on applications. 24-25: Knowing of the principal course arguments, decent speaking ability, limited ability on applications. 21-23: The student has not a full competence of the course arguments but he shows the knowledge, inadequate speaking ability, inadequate ability on applications. 18-20: Inadequate knowing of the course arguments, inadequate speaking ability, very inadequate ability on applications. The examination is considered not sufficient if the student does not show the required minimum knowing of the course arguments.
EDUCATIONAL OBJECTIVES	The "Theoretical and Computational Chemistry" academic course is intended to give the students the fundamental concepts of quantum mechanics and to detail the approaches for their application on chemical problems deriving from the electronic structure of atoms and molecules. The central part of the course deals with the most common methods for the resolution of the polyelectron problem, from the Hartree-Fock method to the density functional theory and the more sophysticated approaches, like coupled cluster. Computer exercises will be done where the methods learned in the frontal lectures are applied to chemical and physico-chemical problems, like the calculation of molecular and spectroscopic properties, the simulation of chemical reactions, approaches for complex systems. The knowing of common softwares for electronic structure calculation is another objective of such exercises.
TEACHING METHODS	Frontal lectures (4CFU, 32 hours), computer exercises (2 CFU, 24 hours)
SUGGESTED BIBLIOGRAPHY	Dispense fornite dal docente (Lecture notes) - Ira N. Levine “Quantum Chemistry” Ed. Prentice Hall - Christopher J. Cramer “Computational Chemistry - Theories and Models” Ed. Wiley. - Attila Szabo, Neil S. Ostlund “Modern Quantum Chemistry - Introduction to Advanced Electronic Structure Theory” Ed. MacMillan Publishing Co.

SYLLABUS

Hrs	Frontal teaching
4	Complementary math: N-dimensional complex vector spaces; eigenvalue equations
4	Basis of quantum mechanics: axiomatic formulation of quantum mechanics; a survey of exactly solvable quantum systems; hydrogenic atoms; atomic orbitals and their properties
4	Introduction to the polyelectron problem: variational theorem; the electron spin; Slater determinants

SYLLABUS

Hrs	Frontal teaching
6	The Hartree-Fock method: derivation and meaning of Hartree-Fock euqations; molecular orbitals; the self consistent field method; basis sets; molecular properties
8	Post-Hartree-Fock methods: the exact wavefunction and the configuration interaction method; the perturbative method; the coupled cluster method
6	Density functional theory: basics; Kohn-Sham equations; the exchange-correlation functionals

Hrs	Practice
6	The molecular geometry optimization; calculation of harmonic vibrational frequencies; simulation of solvent effects; applications
6	Transition states and reaction mechanisms characterization; applications
6	Simulation of NMR spectra: calculation of shielding tensors and coupling constants by means of density functional theory
6	Calculation of spectroscopic constants by means of extremely accurate approaches; applications