UNIVERSITÀ DEGLI STUDI DI PALERMO

DEPARTMENT	Fisica e Chimica - Emilio Segrè
ACADEMIC YEAR	2022/2023
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	8
INDIVIDUAL STUDY (Hrs)	124
COURSE ACTIVITY (Hrs)	76
PROPAEDEUTICAL SUBJECTS	
MUTUALIZATION	
YEAR	1
TERM (SEMESTER)	2° semester
ATTENDANCE	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 matrix 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: - 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 - show adequate speaking ability 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/she 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/she 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. Exercises will be done where some practical issues will be deepened and the methods learned in the frontal lectures are applied, by computer simulations, 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 (5 CFU, 40 hours), exercises (3 CFU, 36 hours)
SUGGESTED BIBLIOGRAPHY	- Dispense fornite dal docente (Lecture notes) - Ira N. Levine “Quantum Chemistry” Ed. Prentice Hall (settima edizione - 2013) - Christopher J. Cramer “Essential of Computational Chemistry - Theories and Models” Ed. Wiley (seconda edizione - 2004)

SYLLABUS

Hrs	Frontal teaching
4	A survey on N-dimensional complex vector spaces
4	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
8	The Hartree-Fock method: derivation and meaning of Hartree-Fock euqations; molecular orbitals; the self consistent field method; basis sets; molecular properties
4	Application of simmetry group theory to the polyelectron problem

SYLLABUS

Hrs	Frontal teaching
10	Post-Hartree-Fock methods: the exact wavefunction and the configuration interaction method; the perturbative method; the coupled cluster method; multiconfigurational and multireference approaches
6	Density functional theory: basics; Kohn-Sham equations; the exchange-correlation functionals

Hrs	Practice
8	Softwares for the calculation of electronic structures: characteristics and peculiarities. Molecular modeling softwares. The Gaussian package: functionality, creation of the input file and reading of the output file. Molecular geometry optimization and calculation of the frequencies of normal modes of vibration; thermochemistry. Equilibrium population of molecular conformations
8	Transition states and reaction mechanisms characterization; applications
8	Simulation of NMR spectra: calculation of shielding tensors and coupling constants by means of density functional theory
12	Computational spectroscopy . Definition of the most importnat molecular spectroscopic constants and their calculation by means of extremely accurate approaches; applications