UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Chimica Fisica Superiore

2223-1-F5401Q027

Aims

Module 1 - Quantum Chemistry

To provide students with the fundamentals of quantum chemistry and present the main methods for calculating structure and properties of molecular systems.

Detailed information is provided in the Syllabus of the Module 1.

Module 2 - Statistical Mechanics

To provide students with the an introduction to statistical mechanics with its chemical applications.

Detailed information is provided in the Syllabus of the Module 2.

Contents

Module 1:
Principles of quantum mechanics. Variation method and perturbation theory. Many-electron atoms. Molecular electronic structure.

Module 2:
Ensembles and phase space. The density of states. The principle of equal a priori probability. Criteria of statistical equilibrium. The Liouville and H theorems. Micro-canonical, canonical and grand-canonical ensembles. Classical and quantum perfect gas.

Detailed program

Module 1
Review of the main principles of quantum mechanics.
Solutions to the Schrödinger equation for many-electron systems: the variation method and the perturbation theory.
Electron spin and antisimmetry.
Many-electron atoms.
Molecular electronic structure: the Born-Oppenheimer approximation; the Molecular Orbital theory. The Hartree-Fock method for MO-LCAO calculations. Example calculations of molecular electronic structures.

Module 2
The equation of motion in the Lagrangian form. Generalised momenta and the canonical equation. Statistical ensembles and the phase space. The density of states. The principle of equal a priori probability. The Liouville theorem. Criteria of statistical equilibrium. Micro-canonical, canonical and grand-canonical ensembles. The Maxwell-Boltzmann distribution for a micro-canonical ensemble. The principle of equipartition. The Boltzmann's H-theorem. Applications: free particles, particles in a box, particles in a harmonic force field, particles with spin. Applications to thermodynamic systems relevant to chemistry: the monoatomic ideal gas, ideal gas mixtures, non-ideal gases. An outline about Bose-Einstein and Fermi-Dirac quantum distributions.

Prerequisites

Basic knowledge of mathematics, physics, quantum mechanics and classical thermodynamics.

Teaching form

The class is made of two sub-units, delivered by Claudio Greco (quantum mechanics) and by Dario Narducci (statistical mechanics), by classroom lectures.
Both sub-units will be delivered through classroom lectures.
Lectures will be in Italian in the absence of Erasmus students; in English otherwise.

Textbook and teaching resource

Module 1:
I.N. Levine, Quantum Chemistry, Prentice Hall; slides from the docent

Module 2:
Reif, Frederick, Fundamentals of statistical and thermal physics, McGraw-Hill, 1965 e Waveland Press, 2009

Semester

First year, first term

Assessment method

Oral exam. Students may opt for partial oral tests, one for each sub-unit. No mid-term test.
The oral exam aims at verifying the level of knowledge acquired, the understanding of the main conceptual junctures in the development of the theory presented during the class and the appropriate use of the language by the student.
The final mark of the course "Advanced Physical Chemistry" is the average of the evaluations obtained in the 2 modules.

Office hours

By appointment

Sustainable Development Goals