UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Chimica Fisica Superiore - Modulo 2

2021-1-F5401Q027-M2

Aims

Aim of this class is to provide students with an introduction to statistical mechanics with its chemical applications

Knowledge and understanding

- Methods of statistical analysis of many-particle systems
- Procedures for the calculation of thermodynamic quantities from microscopic models of many-particle systems
- Basic mathematical tools for the calculation of the partition function
- Methods suitable for the approximate description of classical and quantum interacting systems

Applying knowledge and understanding

- Computation of the equations of state and of the thermodynamic potentials of chemical systems
- Evaluation of the limit of applicability of the classical approximation in chemistry

Making judgements

- Evaluation of the appropriateness of numerical calculation techniques used in commercial simulation codes
- Capbilities of critical analysis of axiomatic scientific theories

Communication skills
Rigorous use of natural language in science

Learning skils
Activation of critical skills in the analysis of scientific models

Contents

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

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

Classical thermodynamics, calculus of functions of several variables, fundamentals of quantum mechanics.

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.

Lectures of statistical mechanics will be delivered partly in the classroom (if allowed) and, for the remaining part, remotely throufìgh Webex. All lectures will be recorded.

Textbook and teaching resource

Semester

First year, first term

Assessment method

Oral exam. Students my opt for partial oral tests, one on each sub-unit. No mid-term tests.

During COVID emergency, the exam will be held online using Webex.

The oral exam aims at verifying the level of knowledge acquired, the understanding of the main conceptual junctures

Office hours

By appointment.