UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

# COURSE SYLLABUS

## Chimica Fisica Superiore - Modulo 2

**2627-1-F5402Q003-2**

### 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 principle of equal a priori probability. Concept of statistical equilibrium. The Liouville and H theorems. Micro-canonical, canonical and grand-canonical ensembles. Classical and quantum perfect gas.

## Detailed program

Elements of descriptive statistics. Representative statistical ensembles and phase space. Postulate of equal a priori probability. Concept of equilibrium in statistical mechanics. Liouville's theorem. Boltzmann's H-theorem. Statistical equivalents of temperature and entropy. Proof of the zeroth, second, and third principles of thermodynamics. Microcanonical, canonical, and grand-canonical ensembles. The Maxwell-Boltzmann distribution in a canonical ensemble. Applications of statistical mechanics: weakly interacting classical and quantum gases. The equipartition theorem.

## Prerequisites

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

## Teaching form

16 two-hour lectures, in person, Delivered Didactics
Lectures will be in Italian in the absence of Erasmus students; in English otherwise.

## Textbook and teaching resource

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 tests.
The oral exam of Statistical Mechanics 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.

## Office hours

By appointment.

## Sustainable Development Goals