UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

# SYLLABUS DEL CORSO

## Complementi di Struttura della Materia

**2122-3-E2701Q061**

### Aims

The aims of this course are to give a first introduction to the classical and quantum statistical mechanics and to provide solid bases of molecular physics also through the theory of finite groups.

### Contents

Elements of classical and quantum statistical mechanics. Introduction to group theory with applications to the study of electronic and vibrational states of polyatomic molecules. Simple molecules: electronic, rotational and vibrational structure.

### Detailed program

1) (KK) chapters 2, 3, 5, 6, 7:

Entropy, temperature and probability.

Canonical ensemble and Boltzmann distribution.

Ideal classic gas.

Chemical potential, grand canonical ensemble and Gibbs free energy.

Quantum statistical distributions: Fermi-Dirac and Bose-Einstein. Classic limit.

Fermi gas.

Low-temperature boson gas and Bose-Einstein condensation, Superfluidity in liquid helium.

Theorem of equipartition and specific heat of polyatomic molecules.

2) (BJ)

Adiabatic approximation.

The MO-LCAO scheme and the secular equation.

Heitler-London and Huckel methods.

The ion and the molecule of hydrogen.

Diatomic molecules.

Vibrational and rotational properties of the diatomic molecule.

The van der Waals molecular interaction.

The Franck-Condon approximation.

3) (AF) chapters 5, 8.7, 10.11-10.12:

Groups and symmetry operations of molecules.

Representation of finite groups, irreducible representations, character table.

Group theory and quantum mechanics, application to the electronic states of polyatomic molecules.

Direct product of two groups. Selection rules of optical transitions in polyatomic molecules.

Vibrations of polyatomic molecules. IR and Raman selection rules.

## Prerequisites

The contents of the mathematics and physics courses of the first two years and of the previous Structure of Matter courses.

## Teaching form

Lectures (in Italian). Textbooks and additional materials may be in both Italian and English.

## Textbook and teaching resource

Suggested textbooks::

(KK) C. Kittel e H. Kroemer, Termodinamica Statistica, Boringhieri (Torino 1985) or the English version, Thermal Physics (W. Freeman, 1980).

(AF) P.W. Atkins and R. S. Friedman, Molecular Quantum Mechanics (5th edition), Oxford University Press (Oxford, 2011); P.W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, Meccanica Quantistica Molecolare (Zanichelli, 2000).

(BJ) B.H. Brandsen e C.J. Joachaim, Physics of Atoms and Molacules, Prentice Hall, 2003

Reccomended books for more informations.

S.J. Blundell and C. Blundell, “Concepts in Thermal Physics” (Oxford University Press, 2009)

D.C. Harris and M. D. Bertolucci, Symmetry and Spectroscopy (Dover, 1989)

## Semester

Second semester.

## Assessment method

The exam consists of a written test and an oral interview. There are no ongoing tests.

The written exam consists in carrying out numerical exercises concerning topics of molecular physics, statistical mechanics and applications of group theory to the electronic and vibrational properties of molecules. During the written test the use of books and notes is not allowed. The grade of the written test is out of thirty and will average

with that of the oral.

The oral exam focuses on the discussion of the theory illustrated during the lectures.

The oral exam must be taken in the same exam session in which the written exam was taken or in the following one.

It is possible, at the request of the student, to take the exam in English.

## Office hours

Every day by appointment.