UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Complementi di Struttura della Materia

2223-3-E2701Q061

Aims

The aims of the course are to give a first introduction to classical and quantum statistical mechanics and to provide a solid foundation 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 canon ensemble and Gibbs distribution.

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

Fermi gas: Fermi energy and specific heat.

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

Photon gas.

Equipartition theorem and specific heat of polyatomic molecules.

2. (BJ)

Adiabatic approximation

The MO-LCAO scheme and the secular equation.

The methods of Heitler-London and Huckel

The ion and the hydrogen molecule

Diatomic molecules

Vibrational and rotational properties of the diatomic molecule

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, table of characters

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 Structure of Matter courses

Teaching form

Frontal lessons held in Italian. Textbooks and additional materials may be in both Italian and English.

Textbook and teaching resource

Suggested texts:

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

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). (AF)

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

For further information:

S.J. Blundell and C. Blundell, "Concepts in Thermal Physics" (Oxford University Press, 200

Semester

Second Semester

Assessment method

The exam consists of a written test and an oral interview.

The written test 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 oral exam focuses on the discussion of the theory illustrated in class.

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

Office hours

Every day by appointment.

Sustainable Development Goals