UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Complements of Atomic and Molecular Physics

2324-3-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. Molecules: electronic, rotational and vibrational structure.

Detailed program

1. Introduction to statistical thermodynamics: (KK) chapters 2, 3, 5, 6, 7:

Entropy, temperature and probability.

Canonical ensemble and the Boltzmann distribution.

Ideal classical gas.

Chemical potential, gran canonical ensemble.

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

Fermi gas: Fermi energy and specific heat.

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

Equipartition theorem and specific heat of polyatomic molecules.

2. Molecular Physics: (BJ)

Adiabatic approximation.

The MO-LCAO scheme and the secular equation.

Heitler-London and Huckel's methods.

The ion and the hydrogen molecule

Diatomic molecules

Organic molecules

Vibrational and rotational properties of molecules

The van der Waals molecular interaction

The Franck-Condon approximation

IR, UV-VIS and Raman spectroscopies

3. Elements of group theory: (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 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 texbooksts:

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

(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). (AF)

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

For in-depth study:

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 next one.

Office hours

Every day by appointment.

Sustainable Development Goals