

## SYLLABUS DEL CORSO

### Struttura della Materia

2526-3-ESM01Q013

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#### Aims

The course aims to provide students with a rigorous and systematic understanding of classical and quantum statistical mechanics, as well as a solid foundation in molecular physics, also integrating elements of finite group theory (Dublin Descriptor 1: Knowledge and understanding). The theoretical framework is designed to foster a critical and informed comprehension of the subject matter and its broader relevance within the field of condensed matter physics.

Through lectures and practical applications, the course aims to strengthen students' ability to independently apply the acquired knowledge to complex problems in molecular and statistical systems, using appropriate theoretical tools and developing suitable mathematical models (Dublin Descriptor 2: Applying knowledge and understanding). Particular emphasis is placed on abstraction, generalization, and knowledge transfer, which are essential for tackling new or interdisciplinary problems.

Finally, the course supports the development of independent learning skills and conceptual tools that enable students to pursue further study or research autonomously, even in highly theoretical or research-intensive contexts (Dublin Descriptor 5: Learning skills).

#### 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. Each theoretical topic will be complemented by an extensive set of exercises designed to reinforce the understanding of key concepts and to develop the ability to apply the theory to model systems and real-world physical situations.

## 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

Diatomc 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.

4. Exercises related to all the above topics.

## Prerequisites

To understand the content of this course, a solid grasp of the main topics covered in the first two years of mathematics and physics is required, particularly the fundamental concepts of quantum mechanics.

## Teaching form

Frontal lessons held in Italian. Textbooks and additional materials may be in both Italian and English. All lectures are given in presence in standard mode (in Italian, the so-called "modalità erogativa") divided into 56 hours of lectures and 36 hours of exercises.

## Textbook and teaching resource

Suggested textbooks:

(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. Branden and C.J. Joachain, *Physics of Atoms and Molecules*, Prentice Hall, 2003 (BJ)

For in-depth study:

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

## Semester

First 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**

QUALITY EDUCATION

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