

# MSE-421 Statistical mechanics

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Cursus	Sem.	Туре	l anguage of	English
Materials Science and Engineering	MA2, MA4		Language of teaching Credits Session Semester Exam Workload Weeks <b>Hours</b>	English 4 Summer Spring Oral 120h 14 <b>4 weekly</b>
			Courses Exercises TP Number of positions	2 weekly 2 weekly 1 weekly 1 weekly

## Summary

This course presents an introduction to statistical mechanics geared towards materials scientists. The concepts of macroscopic thermodynamics will be related to a microscopic picture and a statistical interpretation. Lectures and exercises will be complemented with hands-on simulation projects.

## Content

- From macroscopic thermodynamics to statistical mechanics
- Probability: binomial distribution, central limit theorem, normal distribution
- Ensembles, observables and the partition function
- Examples from materials science
- Undistinguishable particles: Fermi and Bose-Einstein distributions
- Phase transitions: Ising model, spin glasses
- A brief introduction to renormalization group theory
- Theory of liquids structure factor and radial distribution function
- Statistical theories of polymers

## **Keywords**

thermodynamics, statistics, entropy, free energy

## **Learning Prerequisites**

#### Important concepts to start the course

Phenomenological thermodynamics, probability and statistics. A brief "reminder" will be included at the beginning of the course. Practical exercises will be based on Mathematica notebooks: while they are structured in such a way that knowledge of Mathematica programming is not necessary, some familiarity with the software might be useful to go beyond the basic objectives of the exercises.

## Learning Outcomes

By the end of the course, the student must be able to:

- · Compute probabilities of correlated events
- Construct the partition function of simple model systems



- Compare thermodynamic concepts and the correspondent microscopic mechanisms
- Solve simple materials science problems using statistical tools
- Describe the statistical description of liquids and polymers
- Explain the meaning of renormalization group theory
- Conduct computer experiments using the provided simulation code
- Differentiate the meaning of different ensembles, and of the indistinguishability of quantum particles

## **Teaching methods**

Ex cathedra, exercises, and guided simulation projects

## Expected student activities

Students are expected to study demonstrations and fundamental concepts following the course slides and the reference books, to solve the problems given during the exercise sessions, and to prepare (in groups) reports for the computational laboratory activities.

#### **Assessment methods**

Continuous evaluation, graded lab reports, final oral exam

#### Resources

#### **Bibliography**

- E. Fermi, Thermodynamics, Dover
- D. Chandler, Introduction to Modern Statistical Mechanics, Oxford University Press
- K. Huang, Statistical Mechanics
- J. M. Yeomans, Statistical Mechanics of Phase Transitions

#### Ressources en bibliothèque

- Introduction to Modern Statistical Mechanics / Chandler
- Thermodynamics / Fermi
- Statistical Mechanics / Huang
- Statistical Mechanics of Phase Transitions / Yeomans

## **Notes/Handbook**

Comprehensive lecture slides will be provided before each lecture