UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

# COURSE SYLLABUS

# Computational Statistical Thermodynamics in Solids

**2324-1-F1701Q083**

## Aims

The main goal of the Course is to provide to the students some key theoretical/computational tools for approaching at the atomic scale thermodynamics and kinetics of materials.
Notice that this course is called "Computational Materials Science" under the Course in Materials Science and Nanotechnology.

## Contents

Summary of basic concepts in classical statistical mechanics, adiabatic approximation, classical approximation for the motion of nuclei, ab initio and classical molecular dynamics, scientific coding with Matlab, implementation of a molecular dynamics code, application of the molecular dynamics code, configurational Monte Carlo, implementation of a configurational Monte Carlo code, kinetic Monte Carlo, transition state theory.

## Detailed program

Summary of basic concepts in classical statistical mechanics: canonical and microcanonical ensembles. Time averages and microcanonical averages: the ergodic theorem. Thermodynamic limit and equivalence of ensembles,

Adiabatic approximation: nuclear and electronics time scales. Electronic hamiltonian.

Classical treatment of the nuclear motion: nuclear hamiltionian and interatomic potential,

Ab initio vs classical molecular dynamics: semiempirical potentials and their limitations.

Empirical description of the interatomic interactions: pair and manybody potentials. Crystal packing fraction and connection with the choice of the potential.

The Lennard-Jones potential. Introduction of a cutoff and dependence of physical quantities on the cutoff radius.

Introduction to scientific coding, with examples in Matlab. Coding of a function computing the energy of a crystal using Lennard-Jones interatomic potentials. Function for computing neighbors' lists.

Algorithms for integrating the equations of motion: configurational and velocity Verlet. Initial velocities; timestep optimization.

Computing forces in a molecular dynamics code: theory and implementation.

Writing of a complete molecular dynamics code based on Lennard-Jones potentials.

Application of the molecular dynamics code, including additional features such as (a) subtraction of the center of mass momentum (b) rescaling of the initial velocities (c) periodic boundary conditions, to a specific, assigned problem.

The time scale problem: investigating equilibrium configurations via Metropolis Monte Carlo. Writing of a full Metropolis Monte Carlo code.

Application of the Monte Carlo code to a specific, assigned problem.

Advanced topics: (a) temperature control in molecular dynamics using thermostats and/or velocity rescaling (b) thermal cycles/simulated annealing (c) linear-scaling molecular dynamics codes (d) rare events: transition state theory and kinetic Monte Carlo simulations.

## Prerequisites

Basic classical (Boltzmann distribution, isolated systems, systems at constant temperature) and quantum mechanics (wave/particle duality, Schrodinger equation, Pauli esclusion principle).
Knowledge of scientific coding can help but it is not mandatory as dedicated lectures will be given.

## Teaching form

The full course takes places in one of the university informatic laboratories. With the exception of a limited set of initial lectures, each concept is immediately exemplified and elaborated with the help of computer simulations. At half course a first problem is assigned: students are required to solve it by using their first complete (molecular dynamics) code. A second set of lectures follows and a second full (Monte Carlo) code is written and used by the students to solve a second assigned problem. The Course is given in English, but students can ask questions also in Italian.

## Textbook and teaching resource

All lectures, given by the teacher at the informatic laboratory, are accompanied by slides which can be downloaded

from the e-learning platform. While lectures are not taken from a specific text, most topics can be found in Smit and Frenkel book: "Understanding Molecular Simulation: From Algorithms to Applications".

## Semester

First semester (End of September-January)

## Assessment method

The exam is oral only. More specifically:
the two problems assigned during the Course and solved by the students in the informatic laboratory are the subject of the first part of the final exam. Students are required to describe their results with the help of a few slides which the student prepared having in mind a ten minutes presentation for each of the two assigned problems. The teachers evaluates the clarity of the slides and the selection of topics and ask questions on the content. Then a few questions are asked on the general program of the Course, leading to the final mark.

## Office hours

Every day, provided that an appointment is previously fixed by email at least two days in advance.

## Sustainable Development Goals

QUALITY EDUCATION