UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

# SYLLABUS DEL CORSO

## Statistical Thermodynamics of Materials

**2021-2-F5302Q020**

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### 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 solids.

### 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 in Matlab 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 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 using Matlab.

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 and quantum mechanics. Knowledge of the Boltzmann distribution.

## Teaching form

Normally, 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.

Due to the COVID pandemics it is possible that the course will be partially or totally given via distance-teaching through webex or similar platforms. Please check the main elearning page for more information.

## 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 &

Frenkel book: "Understanding Molecular Simulation: From Algorithms to Applications" di Smit & Frenkel.

## Semester

First semester (October-January)

## Assessment method

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.

Due to the COVID Pandemics examinations are presently taking place online, via video-conferences. Changes will be communicated in the main elearning page of the Course.

## Office hours

Every day, provided that an appointment is previously fixed by email.