Computer Simulation of Condensed Matter (SIMCON)

1. Introduction

- Models and force fields

- Simulation methodologies

PART I: MOLECULAR DYNAMICS

2. Solving the equations of motion numerically

- Equations of motion

- Finite Difference Methods: Euler, Verlet, Leapfrog, Runge-Kutta and predictor-corrector algorithms

3. Simulating a system of N particles

- Energies and forces

- Periodic boundary conditions

- Short-range forces and minimum image method

- Long-range interactions: Ewald and reaction field methods

- Thermostats and barostats

- Rigid systems

4. Introduction to quantum methods

- Variational and Hartree-Fock methods

- Density Functional Theory and "ab initio" methods

- Car-Parrinello Molecular Dynamics. Empirical Valence Bond methods. Examples

PART II: MONTE CARLO METHODS

5. Monte Carlo simulation of discrete and continuous systems

- Basics: Metropolis algorithm. Detailed balance

- Monte Carlo statistical ensembles: canonical and beyond

- Re-scaling and finite size phase transitions

PART III: APPLICATIONS

6. Hard Condensed Matter:

- Nanomaterials: carbon nanotubes, graphene

7. Soft Condensed Matter:

- Interfaces and confined fluids: silica pores

- Biomembranes. Interaction with drugs

References:

1. D.Frenkel, B. Smit, ***Understanding Molecular Simulation*****,** Academic Press, 2002.
2. J.M.Thijssen, ***Computational Physics***, Cambridge, 2007.
3. 3. *H.Gould, J.Tobochnik, W.Christian,* ***An Introduction to Computer Simulation Methods: Application to Physical Systems,*** Addison Wesley, 2007.

Qualifying system based on:

A. Questionnaire-exam (20%)

B. Practices with computer (40%)

C. Presentation of personal work (MD or MC project code) in class (40%)

Final mark = 0.2*questions + 0.4*practices + 0.4*Project

A re-evaluation exam will be carried out if necessary.