



Faculté des sciences appliquées

FSA

MAPR2451 Study of materials at the atomic scale

[30h+15h exercises] 4 credits

This course is taught in the 2nd semester

Teacher(s): Vincent Bayot, Patrick Bertrand, Jean-Christophe Charlier, Xavier Gonze (coord.), Luc Piraux
Language: french
Level: 2nd cycle course

Aims

On the basis of numerical simulations, study of materials at the time and space scales corresponding to electronic and molecular phenomena

Main themes

Detailed presentation of simulation techniques valid for all kinds of materials (metals, semiconductors, ceramics, polymers). A series of exercises, tuned towards real materials, allows to apply, thanks to computers, the concepts developed in the Physics of Materials lectures.

Content and teaching methods

Lectures " ex cathedra " : presentation of the concepts

Exercices : the student learns to use different simulation softwares. Then, he/she chooses a topic, studies it, and write a report, that constitutes the main part of the evaluation.

Content of lectures.

A.General presentation of simulation methods

(based on examples, one motivates the use of simulation techniques in material science : very brief, but exhaustive, presentation of different methods ; presentation of physical concepts connected to algorithmic and visualisation techniques, and relations with experimental data)

B.Classical molecular simulations

(empirical or semi-empirical interaction potentials ; molecular dynamics ; search for the equilibrium state ; damped dynamics ; canonical ensemble simulation ; thermostats)

C.Tight-binding simulations

(semi-empirical parametrisation of the hamiltonian ; resolution algorithms ; diagonalisation ; recursion method)

D.Ab Initio simulations

(introduction to Ab Initio techniques ; elements of density functional formalism ; plane wave basis and pseudopotentials ; iterative algorithms)

E.Vibrational and optical properties : theory and simulation

(dielectric tensor, phonons, electronic excitations, photon-phonon interaction, non-linear effects)

Other information (prerequisite, evaluation (assessment methods), course materials recommended readings, ...)

MAPR 2110 Introduction fo materials physics

MAPR 2492 Materials physics