UCL Université catholique de Louvain

LMAPR2451

2012-2013

Study of materials at the atomic scale

5.0 credits	30.0 h + 30.0 h	2q

Teacher(s) :	Charlier Jean-Christophe ; Gonze Xavier (coordinator) ;
Language :	Français
Place of the course	Louvain-la-Neuve
Main themes :	Detailed presentation of simulation techniques valid for all kinds of materials (metals, semiconductors, ceramics, polymers). A series of exercices, tuned towards real materials, allows to apply, thanks to computers, the concepts developed in the Physics of Materials lectures.
Aims :	On the basis of numerical simulations, the student learns to investigate materials at the time and space scales corresponding to electronic and molecular phenomena *The contribution of this Teaching Unit to the development and command of the skills and learning outcomes of the programme(s) can be accessed at the end of this sheet, in the section entitled "Programmes/courses offering this Teaching Unit".*
Content :	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 ; vibrational properties)? Methods : The student learns to use different simulation softwares. Then, he/she chooses a topics, studies it, and write a report, that constitutes the main part of the evaluation. 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 infos :	MAPR 1491 (Supplements in Physics) or a similar course. MAPR 1492 (Materials Physics) or a similar course.
Cycle and year of study :	> Master [120] in Electrical Engineering > Master [120] in Electro-mechanical Engineering > Master [120] in Physical Engineering > Master [120] in Chemical and Materials Engineering
Faculty or entity in charge:	FYKI