UCLouvain

lmapr2451

2024

Atomistic and nanoscopic simulations

5.00 credits	30.0 h + 30.0 h	Q2

Teacher(s)	Charlier Jean-Christophe ;Gonze Xavier ;Rignanese Gian-Marco ;
Language :	English > French-friendly
Place of the course	Louvain-la-Neuve
Main themes	Presentation of nanoscopic scale simulation techniques, based on molecular dynamics, tight-binding and density-functional theory. Considerations related to the speed of execution, numerical accuracy, generality of the techniques, an their intrinsic limitations. Realization of a numerical simulation project of a material. Oral and written presentation of this project and the results, including a critical analysis.
Learning outcomes	**At the end of this learning unit, the student is able to :** 1 **Contribution of the course to the program objectives** Axis Nº1 :1.1, 1.2, 1.3 Axis Nº3 : 3.1, 3.2, and 3.3 Axis Nº4 : 4.1 Axis Nº5 : 5.3, 5.4, 5.5 et 5.6 Axis Nº6 : 6.1, 6.4 **Specific learning outcomes of the course** At the end of their classes, the students are expected to be able: 1. To explain what are the basic principles of different techniques of atomic scale simulations, to use the corresponding software applications, to compare them, and to be able to decide the most appropriate one depending on the properties that must be simulated. 2. To study, indeed, the properties of one material, including the study of the numerical accuracy of results and their validation, and also the comparison with published experimental results, while having a critical view look at the results. 3. To be able to search for scientific information in scientific litterature 4. Present and defend their project orally 5. Write a report on the project, and their results, including the above-mentioned points.
Evaluation methods	Redaction of a report ; oral presentation ; personalized discussion with the teachers.
Teaching methods	Ex cathedra lectures, training sessions with computers, project-based learning, interviews (formative and certificative) with tutors and teachers.
Content	In the firstpart of the course, the lectures, that present the techniques for atomistic and nanoscopic simulations, alternate with training sessions (working on computers), under the supervision of tutors. Some of these exercice sessions are based on tutorials available on the Web. In the second part of the course, students choose and complete a project (individually or in groups of two): • They select a topic of study, and discuss its relevance in a plenary session (at which time a tutor is appointed for their personal coaching); • They study this subject, with regularly consultation of their tutor; • They present the preliminary results at a plenary session; • They then prepare a preliminary report, which is discussed with the teachers during a formative evaluation; • Finally, they submit the report, and defend it in the final certificative evaluation.
Inline resources	Moodle
Bibliography	Disponibles sur Moodle : les directives, les transparents de support.
Other infos	For this lecture, it is assumed that the students have already acquired the basic concepts of materials sciences, quantum physics, statistical physics, and materials physics, taught in bac 2 and in bac 3 (for example, in the lectures LMAPR1805, LMAPR1491, and LMAPR1492), as well as basic notions of computer programming (for example, in the lecture LEPL1401) and of usage of a PC.

Faculty or entity in charge	FYKI

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Learning outcomes
Master [60] in Physics	PHYS2M1	5		🔍
Master [120] in Chemical and Materials Engineering	KIMA2M	5		🔍
Master [120] in Physical Engineering	FYAP2M	5		🔍
Master [120] in Physics	PHYS2M	5		🔍
Advanced Master in Nanotechnologies	NANO2MC	5		🔍