GHENT UNIVERSITY

Course Specifications

Valid as from the academic year 2015-2016

Computational Materials Physics (C003209)

Course size (nominal values; actual values may depend on programme)

Credits	6.0	Study time	180 h
Contact hrs	60.0 h		

Course offerings and teaching methods in academic year 2016-2017

A (semester 1)	Dutch	self-reliant study	20.0 h
		lecture	20.0 h
		guided self-study	20.0 h

Lecturers in academic year 2016-2017

Cottenier, Stefaan	WE05	lecturer-in-charge

Offered in the following programmes in 2016-2017	crdts	offering
Master of Science in Physics and Astronomy	6	A

Teaching languages

Dutch

Keywords

simulations at the atomic scale, DFT, computational materials design

Position of the course

All observable properties of materials are ultimately governed by interactions between their nuclei and electrons. Those interactions are described by the laws of quantum physics. The corresponding mathematical equations that have to be solved, are known since a long time. Thanks to efficient algorithms and ever faster computers, those equations can be effectively solved for an increasing number of situations. In this way, observable properties of materials can be explained directly from quantum physics. In the same way, properties that are not yet measured can be predicted. By hands-on computer exercises, we will learn in this course how to compute many different properties of solids from first principles. Numerous case studies will offer an overview of the computational tools that are available for materials scientists and condensed matter physicists to understand materials at the atomic level -- and even to design them.

Contents

We take a closer look at the method that is most extensively used in this field: density functional theory (DFT). Some implementations of this method are discussed. Then, we'll go through much of the elementary topics in solid-state and materials physics. Most of this has been studied before in other courses, but here we'll look at it from a computational point of view. Emphasis is on learning how to compute condensed matter properties yourself by a state-of-the-art DFT code ("you understand it better once you are able to compute it yourself"). These elementary topics will be linked as much as possible to case studies drawn from the recent research literature. Possible topics are:

- the physics behind the diversity of crystal structures
- relations between crystal structures and observable properties
- predicting elastic properties of crystalline materials
- computing the effect of pressure and predicting pressure-induced phase transitions
- computing the effect of temperature and predicting temperature-induced phase transitions
- computationally predicting phase diagrams
- band structure, and its relation to properties
- understanding and predicting magnetic properties, magnetic phase diagrams
- phonons and derived properties

- electric and thermal conductivity
- doping of semiconductors
- surfaces, interfaces and impurities at surfaces and interfaces
- multiscale modelling: the link between simulations at the atomic level and simulations at the level of the microstructure
- the role of vacancies and how to simulate those
- discovery tools for the focussed design of new materials
- ...

Initial competences

basics of condensed matter physics and/or materials science, basics of quantum physics

Final competences

1 Being able to explain the concepts behind density-functional theory.
2 Using a general-purpose density-functional theory code to calculate basic properties of a given solid.
3 Evaluating the precision and accuracy of a density-functional theory prediction for a given solid and given property.
4 Being able to understand and to critically evaluate research literature in which density-functional theory results are reported.
5 Formulating a strategy to use density-functional theory to address a materials problem.

Conditions for credit contract

Access to this course unit via a credit contract is determined after successful competences assessment

Conditions for exam contract

This course unit cannot be taken via an exam contract

Teaching methods

Guided self-study, lecture, self-reliant study activities

Extra information on the teaching methods

The emphasis of this course is on action: you will not be taught (passive), you will learn (active). This will be realized in various ways:
- all exercises will be made on the **high-performance computing** infrastructure of Ghent University. You can do this at home as well as during sessions dedicated to this.
- most topics will be offered in a **flipped classroom** model: you watch at home a set of videos on the topic, you submit a report with your answers to the questions/tasks related to these videos, and in the next class session we discuss the problems you might have encountered while doing so.
- In a team of 3-4 students you will work during the entire semester on a **project**, applying the methods you learn during the course.

It will be tried to initiate interaction and collaboration with students from other universities/countries that are taking a similar course.

Learning materials and price

All learning materials (15 hours of dedicated video files plus text files) are available on a digital learning platform. Cost: 0 euro.

References

- Density Functional Theory: a practical introduction (D.S. Sholl, J.A. Steckel, Wiley 2009)
- Electronic structure – basic theory and practical methods (R. M. Martin, Cambridge 2004)
- Computational Materials Science: from basic principles to material properties (W. Hergert, A. Ernst, M. Däne (ed), Springer 2004)
- Atomistic Computer Simulations: A Practical Guide (V. Brazdova, D.R. Bowler, Wiley 2013)
- Understanding Solids: the science of materials (Richard J. D. Tilley, John Wiley & Sons, 2013)

Course content-related study coaching

Evaluation methods

end-of-term evaluation and continuous assessment

Examination methods in case of periodic evaluation during the first examination period

Written examination, open book examination, oral examination, skills test

Examination methods in case of periodic evaluation during the second examination period

Written examination, open book examination, oral examination, skills test

Examination methods in case of permanent evaluation

Participation, skills test, peer assessment, report

Possibilities of retake in case of permanent evaluation

examination during the second examination period is possible in modified form

Extra information on the examination methods

- You are expected to submit weekly a report with your answers to the questions/tasks of that week. Your effort in doing so will be evaluated, not the correctness of your answers.
- As member of a team, you will work throughout the course on a project: studying a materials problem by computational methods. Near the end of the semester, each team will submit a 'research paper' and will give a 'conference presentation' to communicate your results.
- The exam will be a combination of written and oral questions, combined with a (short) task that has to be performed on the computer. This exam is open book.

Calculation of the examination mark

- weekly report: 20% (per non-submitted report, 5% is subtracted - with a floor of 0%)
- project: 40%
- exam: 40%

You have to pass on the combined items 'project' and 'exam' in order to pass for the course. In case you don't pass the project+exam (e.g. 7/16) then your points obtained for the weekly reports (e.g. 3/4) are added only to a maximum of 9 (e.g. 7+2=9, 1 point is discarded).