GHENT UNIVERSITY

Course Specifications

Valid in the academic year 2022-2023

Computational Materials Physics (E024121)

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

Credits 6.0 **Study time 180 h** **Contact hrs** 60.0h

Course offerings and teaching methods in academic year 2022-2023

A (semester 1)	Dutch	Gent	project	0.0h
			lecture: response lecture	15.0h
			guided self-study	0.0h
B (semester 1)	English	Gent	lecture: response lecture	15.0h
			project	0.0h
			guided self-study	0.0h

Lecturers in academic year 2022-2023

Cottenier, Stefaan	TW08	lecturer-in-charge

Offered in the following programmes in 2022-2023	crdts	offering
Master of Science in Teaching in Science and Technology(main subject Physics and Astronomy)	6	B
European Master of Science in Nuclear Fusion and Engineering Physics	6	B
Master of Science in Materials Engineering	6	A, B
Master of Science in Physics and Astronomy	6	B
Master of Science in Sustainable Materials Engineering	6	B

Teaching languages

English, Dutch

Keywords

simulations at the atomic scale, materials physics, 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 the course how to compute many different properties of solids from first principles. 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 first a closer look at the method that is most extensively used in this field: density functional theory (DFT). After a survey of the large number of available DFT codes, we start hands-on work with one of those codes (a free and open source code : everything you learn here, you can keep using later on). Step by step, you learn how to use DFT to predict basic properties of crystalline materials: geometrical, electronic, elastic and chemical properties. Furthermore, you'll learn how to assess the reliability of your predictions, ánd of the (not always reliable) predictions you meet in the scientific literature.

Initial competences

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

Final competences

1 Using a general-purpose density-functional theory code to calculate basic properties of a given solid.
2 Being able to explain the concepts behind density-functional theory.
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, Project, Lecture: response lecture

Extra information on the teaching methods

- This course is offered via **flipped classroom** : every week, 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 weekly feedback webinar we discuss the problems you might have encountered while doing so. It is your choice whether you attend this feedback session in the lecture room, via a livestream, or whether you watch a recorded version later.
- **'do it yourself'** is important in this course: you learn step by step how to use a DFT code to predict materials properties. You can run the code on your own laptop. For calculations that require more computing time, you have access to the high-performance computing environment of Ghent University.
- You get the chance to work in a team of 3-4 students during the entire semester on a **project**, applying the methods you learn during the course.
- This course is accessible as an open online course for anyone, **worldwide**. Whenever possible, we try to establish interactions between students in Ghent and volunteering participants on other continents.

Learning materials and price

All learning materials (15 hours of dedicated video files plus text files) are available on www.compmatphys.org. 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

During the weekly feedback webinar, questions that were submitted during the preceding week are collectively addressed. The hour following the feedback webinar is reserved for students with specific questions that are less suitable for collective feedback.

Assessment moments

end-of-term and continuous assessment

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

Skills test, Written examination, Oral examination, Open book examination

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

Skills test, Written examination, Oral examination, Open book examination

Examination methods in case of permanent assessment

Skills test, Report, Participation, Peer assessment

Possibilities of retake in case of permanent assessment

examination during the second examination period is possible in modified form

Extra information on the examination methods

- You 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.
- You can opt for an "assessment via a project". 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 written report in the form of a paper for an (imaginary) scientific journal, and an oral report in the form of a 5-minute video. If you take this evaluation method, you have a higher work load throughout the term, yet a lighter examination period.
- Alternatively, you can opt for an "assessment via an exam". 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 and open internet. If you take this evaluation method, then the work load throughout the term is lower, yet you have an additional exam during the examination period.

Calculation of the examination mark

- weekly report: 20% (per non-submitted report, 5% is subtracted - with a floor of 0%)
- if one choses the option 'project': 80% (based on the written report and the video report, and this as well by the lecturer as via peer evaluation among teams and within each team -- not every team member will necessarily have the same result)
- if one choses the option 'exam': 80%

If one passes the item 'project' or 'exam', then the grade for project/exam and the grade for the weekly tasks are added unconditionally. If one does not pass on project/exam, then the grade for the weekly tasks is added to the grade for project/exam with a cap of 45% (example: 6/16 for the exam and 4/4 for the weekly tasks would lead to a sum of 10/20. As this student did not pass the item 'exam', only 3 points are added from the grade on the weekly task, as with 6+3=9 the ceiling of 45% (9/20) is reached).

Facilities for Working Students

All lecture content is permanently available under the form of prerecorded videos. The weekly feedback webinars are live-streamed and recorded.