GHENT UNIVERSITY

Course Specifications

Valid as from the academic year 2024-2025

Computational Materials Physics (E024122)

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

Credits 6.0 **Study time 180 h**

Course offerings in academic year 2024-2025

A (semester 2)	English	Gent
B (semester 1)	English	Gent
C (semester 2)	Dutch	Gent

Lecturers in academic year 2024-2025

Cottenier, Stefaan	TW08	lecturer-in-charge
Kestens, Leo	TW08	co-lecturer

Offered in the following programmes in 2024-2025	crdts	offering
Master of Science in Teaching in Science and Technology(main subject Physics and Astronomy)	6	B
Bridging Programme Master of Science in Sustainable Materials Engineering	6	A
European Master of Science in Nuclear Fusion and Engineering Physics	6	A
Master of Science in Materials Engineering	6	C
Master of Science in Physics and Astronomy	6	B
Master of Science in Physics and Astronomy	6	B
Master of Science in Sustainable Materials Engineering	6	A

Teaching languages

English, Dutch

Keywords

simulations at the atomic scale, materials physics, DFT, computational materials design

Position of the course

Observable properties of materials are determined by physical phenomena at various length scales. At the quantum scale, the interaction between nuclei and electrons determines the chemical bonds, which in turn lead to, for instance, a specific crystal structure, compressibility or color of the material. At the microscopic scale, the material properties are determined by the collective behavior of lattice defects such as vacancies, dislocations or grain boundaries. Mathematical equations to describe these phenomena are known for a long time. These can be first principles expressions (quantum scale), phenomenological or thermodynamic expressions at the micro scale. 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 and/or predicted by simulations, prior to doing experiments. By hands-on computer exercises, you will learn in this course how to compute different properties of solids at one or more length scales. 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 above -- and even to design them.

Contents

Following a global discussion of the typical aspects of simulations at the quantum scale vs. simulations at the microscale, you will be introduced to the workhorse method for quantum simulations: density functional theory (DFT). This includes right from the start hands-on work with a DFT code. The code is free and open source, which guarantees that you can keep using it later in your education, research or job. We'll focus first on predicting structural properties of crystalline materials. At this point the course bifurcates and you can choose one of these two tracks: continuing with simulations at the quantum scale for electronic, magnetic and other properties of crystals, or stepping up to the microscale for simulations of a different kind about structural dependent properties or microstructural evolutions.

Initial competences

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

Final competences

1 Being able to explain the concepts behind density-functional theory and the major simulation strategies at the micro scale.
2 Using a general-purpose density-functional theory code to calculate basic properties of a given solid.
3 Being able to understand and to critically evaluate research literature in which the simulation methods used in this course are applied.
4 Evaluating the precision and accuracy of different simulation methods for a given solid and given property.
5 Formulating a sound simulation strategy 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

Lecture, Independent work

Extra information on the teaching methods

- This course is mainly 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, and you have the chance to program your own microstructure simulation model. You can run these codes 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.

Study material

None

References

- Dierk Raabe, "Computational Material Science", Wiley-VCH, 1998, ISBN- 3-527-29541-0Density 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)
- "Introduction to Materials Modelling", edited by Zoe H. Barber, 2005, Published by The Institute of Metals, London, ISBN 1-902653-58-0

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, Oral assessment, Written assessment

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

Skills test, Oral assessment, Written assessment

Examination methods in case of permanent assessment

Skills test, Participation, Peer and/or self assessment, Assignment

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

- When you follow the quantum scale track (half of the course or the entire course), 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. If you follow the microscale simulation track in the second half of the course, the weekly task reports are replaced by reporting on your project progress.
- You can opt for an "assessment via a project" in the quantum scale track, whereas for the microscale track this is the default assessment method. This means 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" (only possible for the quantum scale track). 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 an oral one-on-one discussion, on the written report and on 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% (only possible within the quantum scale track)

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