GHENT UNIVERSITY

Course Specifications

Valid in the academic year 2023-2024

Modelling and Engineering of Nanoscale Materials (E006800)

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

Credits 6.0 **Study time 180 h**

Course offerings and teaching methods in academic year 2023-2024

A (semester 1)	English	Gent	lecture seminar
B (semester 1)	Dutch	Gent	

Lecturers in academic year 2023-2024

Vanduyfhuys, Louis	TW17	lecturer-in-charge
Rogge, Sven	TW17	co-lecturer

Offered in the following programmes in 2023-2024	crdts	offering
Master of Science in Teaching in Science and Technology(main subject Physics and Astronomy)	6	A
European Master of Science in Nuclear Fusion and Engineering Physics	6	A
Master of Science in Engineering Physics	6	B
Master of Science in Engineering Physics	6	A
Master of Science in Materials Engineering	6	B
Master of Science in Physics and Astronomy	6	A
Master of Science in Sustainable Materials Engineering	6	A
Exchange Programme in Physics and Astronomy (Master's Level)	6	A

Teaching languages

English, Dutch

Keywords

many-body physics, interatomic interactions, molecular dynamics, electronic-structure theory, spectroscopy, basis sets for wavefunctions, force fields, nanoscale materials design, electronic engineering (energy conversion, luminescence), mechanical engineering (shock absorbers, mechanical sensors), thermal engineering (thermal conductors, heat reservoirs), structure characterization and prediction

Position of the course

Engineering applications rely more and more on highly specialized materials exhibiting unique functionalities. In recent years, for example, advanced functional materials such as hybrid perovskites, metal-organic frameworks, and covalent organic frameworks have proven invaluable to overcome many of the challenges associated with the development of high-performance photovoltaics, efficient heat management systems or stimulus-responsive sensor materials. The rational design of such advanced functional materials requires insight at the atomic level. In this respect, molecular modelling is an interdisciplinary field that allows gaining information on the physical phenomena that govern the behaviour of these materials at the nanoscale. It has attracted increasing interest due to the systematically growing computer capabilities and the continuous optimization of physical models and numerical algorithms. The application fields are very diverse, going from chemistry, molecular physics, solid-state physics, and materials physics to nanophysics.

In this course, nanoscale modelling techniques are introduced by building upon

concepts from quantum mechanics, statistical physics, and atomic and molecular physics, focusing on the applicability of these concepts and the rational approximations necessary to model real-life nanostructured materials with industrial relevance. To model these nanosized functional materials, a variety of simulation techniques are discussed and applied in this course. These modelling techniques vary from quantum mechanics based methods, which are ideally suited to study complex nanosystems of limited sizes or at restricted time scales, to classical force field based methods, which are able to describe phenomena taking place on the microsecond scale in systems of several tens of nanometers in size. These techniques are then applied to study structural, mechanical, spectroscopic, and thermal properties of molecules and solids. The course focuses on the development of functional materials for engineering applications in the conversion and storage of energy, the sensing of chemical and physical stimuli, and heat management on the nanoscale. The student will learn to work with different software packages which are commonly used in scientific research.

Contents

The most common strategy to model nanoscale systems is to apply the Born-Oppenheimer approximation, in which the electronic and nuclear degrees of freedom are decoupled. The energy of the system then reduces to a parametric function of the position of the atomic nuclei. The resulting multidimensional energy hypersurface is referred to as the potential energy surface (PES) and governs the structural flexibility of the considered material. This course demonstrates how the PES can be constructed from quantum mechanical information (electronic-structure methods) or more approximate techniques (force fields), and how adequate sampling of the PES allows recovering macroscopic properties of the material. These methods are used to gain insight into materials behaviour at the nanoscale and develop design strategies based on atomic information.

The course consists of the following main parts:

1 Introduction to molecular modelling: typical engineering applications, typical time and length scales, interatomic interactions
2 Sampling techniques to derive macroscopic properties from the potential energy surface: normal-mode analysis, partition functions, molecular dynamics, rare-event sampling schemes, Monte Carlo approaches, vibrational spectroscopy
3 Many-body electronic-structure methods: Hartree-Fock, post-Hartree-Fock, density-functional theory, electronic spectroscopy
4 Basis sets for the description of electronic states: localized basis sets, plane-wave basis sets, pseudopotentials, projector-augmented wave method
5 Molecular mechanics to model larger systems on longer time scales: force field methods, atom-in-molecule partitioning
6 First-principles materials design to rationally identify materials with outstanding performance in, for instance thermal engineering (thermal conductivity, heat capacity), mechanical engineering (elastic constants, structural flexibility), electronic engineering (band gap, charge carrier mobility, UV/visible/infrared spectrum)

Initial competences

This course builds upon certain final competences from quantum mechanics, statistical physics and atomic and molecular physics.

Final competences

1 Understand the nanoscale composition of engineering materials and the physical interactions within.
2 Master basic concepts and terminology with respect to modelling nanoscale materials.
3 Determine the most suitable models and approximations to describe the interactions governing macroscopic thermal, mechanical, and electronic behaviour of advanced materials.
4 Start from theoretical concepts at the nanometer scale and numerical aspects to engineer materials for targeted applications.

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

Seminar, Lecture, Independent work

Extra information on the teaching methods

Classroom lectures; Computer-assisted problem solving with own laptop, where state of the art modeling programs commonly used in this research discipline are used.

Learning materials and price

Slides

References

- D. Frenkel and B. Smit, Understanding Molecular Simulation: From Algorithms to Applications, Academic Press, 2nd edition, 2002.
- R. Parr and W. Yang, Density-Functional Theory of Atoms and Molecules, Oxford University Press, 1989.
- R. Martin, Electronic Structure: Basic Theory and Practical Methods, Cambridge University Press, 2004.
- E. R. Leite, Nanostructured Materials for Electrochemical Energy Production and Storage, Springer, 2009.
- A. Fereidoon, M. D. Ganji, F. Memarian, and M. Dehghan, Mechanical Properties of Nanostructured Materials: Quantum Mechanics and Molecular Dynamics Insights, Xlibris Us, 2016.
- P. Sanghera, Quantum Physics for Scientists and Technologists: Fundamental Principles and Applications for Biologists, Chemists, Computer Scientists, and Nanotechnologists, Wiley Interscience, 2011.

Course content-related study coaching

Teacher and assistants are available for questions during or between classes or by appointment; support is foreseen during the exercise sessions.

Assessment moments

end-of-term assessment

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

Oral assessment, Assignment

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

Oral assessment, Assignment

Examination methods in case of permanent assessment

Possibilities of retake in case of permanent assessment

not applicable

Extra information on the examination methods

- Evaluation by project (grading of participation in the project, project report and oral presentation) and oral examination.
- Second chance: Possible in adapted form.

Calculation of the examination mark