Course Specifications

Valid as from the academic year 2015-2016

Simulations and Modelling for the Nanoscale (E023370)

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)	lecture	30.0 h
	seminar: practical PC room classes	30.0 h

Lecturers in academic year 2016-2017

Van Speybroeck, Veronique	TW17	lecturer-in-charge
Lejaeghere, Kurt	TW17	co-lecturer

Offered in the following programmes in 2016-2017	crdts	offering
Elective Course List European Master of Science in Nuclear Fusion Science and Engineering Physics	6	A
Master of Science in Physics and Astronomy	6	A
European Master of Science in Nuclear Fusion and Engineering Physics	6	A
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 Engineering Physics	6	A
Exchange Programme in Physics and Astronomy (master's niveau)	6	A

Teaching languages

English

Keywords

many-body systems, supramolecular systems, Hartree-Fock, density functional theory, basis sets, pseudopotentials, plane waves, molecular dynamics, spectroscopy, nanophysics

Position of the course

Molecular Modeling is an interdisciplinary field with increasing interest due to the systematically growing computer capabilities, and the continuous optimization of physical models and available numerical algorithms. The application fields are very divers, going from chemistry, molecular physics, solid-state physics, material physics to nanophysics. Theoretical modeling offers a powerful tool to study all features which take place on the nanoscale. In particular the non-covalent interactions between molecules in a supramolecular system belong to the topics of this lecture. Solving the quantummechanical many-electron problem lies on the basis of all applications: determination of the stable geometry of the system and other conformational structures, evaluation of molecular properties, such as the kinetics of chemical reactions, spectroscopic quantities (IR, NMR), semi-conductor characteristics, catalytic behavior, etc. Pure quantummechanical approaches are not always feasible to tackle all phenomena, and it depends on the time scale of the observed phenomena whether classical or hybrid methods are more adequate. Molecular dynamics is a powerful tool to study macroscopic behaviors.
In this course, theoretical methods are presented that are available for the study of nanoscale systems. The student learns to work with different software packages which are commonly used in scientific research.

Contents

- Interactions present at the nanoscale: bonding, non-bonding, electrostatic, Van Der

Waals interactions
- Born-Oppenheimer approximation for molecular systems
- Techniques to determine the electronic structure: independent particle model, Hartree-Fock concept, post-Hartree-Fock methods, Density Functional Theory, semi-empirical methods, molecular mechanics
- Basis set: localized Gaussian basis sets, plane-wave pseudopotential methods, combined Plane Wave and localized basisset implementation (GPW)
- Molecular dynamics: classical molecular dynamics, force fields, Car-Parrinello molecular dynamics
- Hybrid calculation methods: embedding schemes for supramolecular systems, QM/MM methods, discrete solvatation or continuous embedding
- Spectroscopy: vibrational analysis (IR/Raman), calculation of thermodynamic properties, reaction kinetics, electronic spectroscopy (UV/Vis)
- Applications: molecular modelling with computer packages (Gaussian09, CP2K, CPMD, VASP,...), conformational analysis of molecular systems, clustermodels in crystals, electronic structure and properties of polyaromatics, geometric, electronic and spectroscopic properties of defects in crystals, adsorption properties in porous materials, structure characterization organic solvents, nanostructure of materials

Initial competences

Quantummechanics, Statistical Physics

Final competences

1. Concepts: many body techniques, interactions on the nanoscale, Hartree-Fock formalism, density functional theory, classical force fields, molecular dynamics, hybrid schemes, supramolecular systems, spectroscopy, nanophysics.
2. Insights: insight in the most important interactions playing at the nanoscale; insight in the most important computational methods to describe molecular systems with a length scale of about 0.1 to 10 nm; insight in approximations and applicability of molecular models and methods.
3. Skills: be able to apply various computer packages to model a molecular system; for a given molecular problem be able to design a suited computationally efficient technique; knowing important applications of computational nanophysics.

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, seminar: practical PC room classes

Extra information on the teaching methods

Classroom lectures; Computer-assisted problem solving; Classroom problem solving sessions

Learning materials and price

Syllabus

References

- R.Parr and W.Yang, Density Functional Theory
- Plane waves, pseudopotentials and the LAPW method, D.J. Singh, Kluwer Academic Publishers, 1994.

Course content-related study coaching

Evaluation methods

continuous assessment

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

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

Examination methods in case of permanent evaluation

Oral examination, assignment

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

Evaluation by project: grading of project report; grading of oral presentation and examination.
Second chance: Possible in adapted form.

Calculation of the examination mark