

## 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
<a href="#">Elective Course List European Master of Science in Nuclear Fusion Science and Engineering Physics</a>	6	A
<a href="#">Master of Science in Physics and Astronomy</a>	6	A
<a href="#">European Master of Science in Nuclear Fusion and Engineering Physics</a>	6	A
<a href="#">Master of Science in Sustainable Materials Engineering</a>	6	A
<a href="#">European Master of Science in Nuclear Fusion and Engineering Physics</a>	6	A
<a href="#">Master of Science in Engineering Physics</a>	6	A
<a href="#">Exchange Programme in Physics and Astronomy (master's niveau)</a>	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 diverse, 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 basis set 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 solvation 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, cluster models 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**