GHENT UNIVERSITY

Course Specifications

Valid as from the academic year 2024-2025

Molecular Physical Chemistry (C004128)

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 2024-2025

A (semester 1)	English	Gent	seminar
			lecture

Lecturers in academic year 2024-2025

Hens, Zeger	WE06	lecturer-in-charge
De Proft, Frank	VUB	co-lecturer
Schiettecatte, Pieter	WE06	co-lecturer

Offered in the following programmes in 2024-2025	crdts	offering
Master of Science in Teaching in Science and Technology(main subject Chemistry)	6	A
Master of Science in Chemistry(main subject (Bio)Organic and Polymer Chemistry)	6	A
Master of Science in Chemistry(main subject Materials and Nano Chemistry)	6	A
Exchange Programme in Chemistry (master's level)	6	A

Teaching languages

English

Keywords

Position of the course

The course makes students understand that the combination of molecular theory and physical laws provides the most fundamental understanding of chemical phenomena. The course aims at an understanding of the concepts that scientists use to relate molecular properties to macroscopic quantities, with a particular emphasis on statistical thermodynamics (equilibrium) and molecular reaction dynamics (change). This conceptual framework is complemented by a practical introduction in state-of-the-art methods to model molecular properties, encompassing density functional theory and molecular dynamics. This combination of conceptual understanding and computational skills serves to deepen the knowledge in molecular physical chemistry and will enable students to apply the general principles to practical problems.
The modules (1) concepts in molecular physical chemistry and (2) molecular modelling can be followed as Advanced Topics in Chemistry.

Contents

Concepts of Molecular Physical Chemistry

1 The quantum mechanical view on the physical world.
2 The concepts of statistical mechanics.
3 The statistics of non-interacting particles.
4 Statistical thermodynamics of the ideal gas.
5 Lattice models.
6 Molecules in solvents - fluctuations and transport.
7 Moleculaire reaction dynamics.
8 Transition state theory.

Introduction to Molecular Modelling

1 Practical introduction to electronic structure methods with particular attention for density functional theory

2 Computation of the electronic structure and interpretation of the results.
3 Geometry optimization: minima and saddle points (transition states).
4 Computation of spectroscopic quantities: electronic transitions, vibrational frequencies and NMR properties.
5 ab initio molecular dynamics: dynamic properties and solvent effects.

Initial competences

Students are familiar with mathematical concepts for chemists and have followed courses in chemical thermodynamics and quantum chemistry.

Final competences

1 Students have quantum mechanical insight in the optical and electronic properties of molecules and in intermolecular interactions.
2 Students can model optical and electronic properties of molecules through density functional theory.
3 Students can explain the concepts of statistical thermodynamics.
4 Students can apply statistical thermodynamics to the analysis of systems of non-interacting particles.
5 Students can interpret properties of thermodynamic systems by the use of lattice models.
6 Students understand the behavior of molecules in solvents, they can model this behavior through molecular dynamics and relate this behavior the physical transport processes.
7 Students understand the principles of moleculaire reaction dynamics and can link molecular reaction dynamics to transition state theory.
8 Students have a qualitative insight in potential energy surfaces and can link it to elementary reaction pathways.
9 Students can independently perform state-of-the-art density functional calculations of different properties and can correctly interpret the results.

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

- **Lecture** - will be used to teach students the concepts of statistical thermodynamics and molecular models on physical and chemical kinetics
- **Seminars** - will be used to teach students the concepts of statistical thermodynamics and molecular models on physical and chemical kinetics
- **Guided self-study** - on-line knowledge clips will be used to introduce students in the theory underlying molecular modelling
- **Integration Seminar** - will be used to train students in the practical use of molecular modelling tools

Study material

Type: Syllabus

Name: Syllabus'
Indicative price: € 15
Optional: no

References

Course content-related study coaching

Assessment moments

end-of-term assessment

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

Oral assessment, Written assessment, Assignment

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

Oral assessment, Written 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

- **Assignment** - evaluation of the exercises in statistical thermodynamics and the part on molecular modelling. Assignments will be distributed by December 1. The report will be defended orally as part of the periodic evaluation.
- **Oral/Written exam** - evaluation of the theory part of concepts of molecular physical chemistry.

Calculation of the examination mark

- **Assignmen** - 11/20
- **Oral/Written examn** - 9/20