GHENT UNIVERSITY

Course Specifications

From the academic year 2015-2016 up to and including the

Molecular Physical Chemistry (C002547)

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

Credits	6.0	Study time	180 h	Contact hrs	45.0 h

Course offerings and teaching methods in academic year 2018-2019

A (semester 1)	English	seminar: coached exercises	20.0 h
		lecture	27.5 h

Lecturers in academic year 2018-2019

Hens, Zeger	WE06	lecturer-in-charge

Offered in the following programmes in 2018-2019	crdts	offering
Master of Science in Chemistry	6	A
Exchange Programme in Chemistry (master's level)	6	A

Teaching languages

English

Keywords

statistical thermodynamics, lattice models, physical transport, chemical reaction dynamics

Position of the course

Molecular physical chemistry is a compulsory course in the masters in chemistry program. It is based directly on the mathematics, physics and physical chemistry (including quantum chemistry) courses at the bachelor level and provides a qualitative background for the molecular modelling course in the masters in chemistry program. 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 a qualitative understanding of concepts. Emphasis is lead on statistical thermodynamics (equilibrium) and molecular reaction dynamics (change). The course adresses the following competences: M.1.1, M.1.3, M.1.4, M.2.2, M.3.4, M. 3.5, M.3.6, M.4.1, M.4.3, M.6.2.

Contents

1. The quantum mechanical view on the physical world.
2. An overview of probability and statistics.
3. The concepts of statistical mechanics.
4. The statistics of non-interacting particles.
5. Statistical thermodynamics of the ideal gas.
6. Electrical and optical properties of molecules.
7. Lattice models.
8. The concept of temperature - fluctuations.
9. A molecular view on physical transport .
10. Moleculaire reaction dynamics.
11. Transition state theory.
12. Qualitative models for the potential energy surface.

Initial competences

Students need to have obtained credits for the following courses in the chemistry curriculum or have successfully followed other courses with a similar content: “Applied Mathematics for Chemists”, “Physical Chemistry I: Chemical Thermodynamics”, “Physical Chemistry II: Electrochemistry, Chemical Kinetics” 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 explain the concepts of statistical mechanics.
3 Students can apply statistical mechanics to the analysis of systems of non-interacting particles.
4 Students can interpret properties of thermodynamic systems by the use of lattice models.
5 Students understand the concept of temperature and can relate temperature and the occurence of fluctuations by using statistical thermodynamics.
6 Students can explain physical transport from a molecular point of view.
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.

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: coached exercises

Learning materials and price

English language course book. Cost: 15 EUR

References

Ken A. Dill, Sarina Bromberg, Molecular Driving Forces, Garland Science, New York, 2003.

Course content-related study coaching

Interactive support by means of Minerva. Possibility for questions and discussions following each classroom lecture.

Evaluation methods

end-of-term evaluation

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

Written examination with open questions, written examination, open book examination, oral examination, report

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

Written examination with open questions, written examination, open book examination, oral examination, report

Examination methods in case of permanent evaluation

Possibilities of retake in case of permanent evaluation

examination during the second examination period is possible

Extra information on the examination methods

The evaluation consists of two parts, covering theory and exercises.

Calculation of the examination mark

theory: 12/20
exercises: 8/20