Course Specifications

Valid as from the academic year 2016-2017

Computational Chemistry (C002550)

Course

Valid as from the academic year 2016-2017

Course size

<table>
<thead>
<tr>
<th>Credits</th>
<th>Study time</th>
<th>Contact hrs</th>
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<tbody>
<tr>
<td>6.0</td>
<td>170 h</td>
<td>64.5 h</td>
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Course offerings and teaching methods in academic year 2017-2018

A (semester 2)

lecture: 22.5 h

seminar: practical PC room classes 45.0 h

Lecturers in academic year 2017-2018

Bultinck, Patrick WE06 lecturer-in-charge

De Proft, Frank VUB co-lecturer

Van Damme, Sofie WE06 co-lecturer

Offered in the following programmes in 2017-2018

Master of Science in Chemistry 6 A

Exchange Programme in Chemistry (master's level) 6 A

Teaching languages

English

Keywords

Computational chemistry, Molecular Modelling

Position of the course

The aim of this course is to provide an introduction in the broad and diverse field of computational chemistry and to give an overview of its different important topics and subdisciplines. This course thus provides the necessary background to read research papers in this area and should allow the students to critically assess the quality of computational studies and to put them in proper perspective. Also, the students learn to individually choose and apply an adequate methodology to tackle research problems in computational chemistry.

Contents

• Introduction : Computational chemistry
• Force Field Methods
• Electronic structure methods
• Electron correlation
• Introduction to Density Functional Theory
• Basis sets
• Reactivity and QSAR
• Response properties
• Qualitative theories

Initial competences

Bachelor of Science in Chemistry, Physics, Bio-engineering or Engineering. A number of introductory chapters will be provided for guided self-study if no previous courses in quantum mechanics or quantum chemistry have been taken.

Final competences

1 The student gains knowledge and insight into different computational chemistry topics and techniques to investigate the properties of chemical systems.
2 The student is able to judge the quality of published computational studies.
3 The student is able to select the proper methods for a problem at hand.
4 The student is able to apply computational chemistry methods in a broader chemical environment.

(Approved)
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
The seminars (WPO) consist of a number of computer exercises in order to better digest the theory and to apply it to concrete chemical problems.

Learning materials and price
The slides used during the lectures will be available for the students through the electronic learning platforms of the UGent and the VUB. The textbook "Introduction to Computational Chemistry" by F. Jensen (Wiley) is advised.

References
"Introduction to Computational Chemistry" by F. Jensen (Wiley)

Course content-related study coaching
Guidance by lecturer and assisting staff during computer classes and on appointment.

Evaluation methods
end-of-term evaluation and continuous assessment

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

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

Examination methods in case of permanent evaluation
Report

Possibilities of retake in case of permanent evaluation
not applicable

Extra information on the examination methods
1. During the PC classes the students get one or more assignments per class on which they prepare a written report which is assessed and marked as part of the non-periodic evaluation.
2. The rest of the grade is obtained from the result of the written examination, in which the knowledge and insight of the student into the course material is evaluated.

Calculation of the examination mark
50% of the end score is based on the non-periodic evaluation. Failure to submit the reports within the deadline set, renders a zero score for this report. The remaining 50% is based on the periodic evaluation.