Course Specifications
Valid as from the academic year 2016-2017

Quantum Chemical Methods (C002962)

Course size

<table>
<thead>
<tr>
<th>Credits</th>
<th>Study time</th>
<th>Contact hrs</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.0</td>
<td>90 h</td>
<td>30.0 h</td>
</tr>
</tbody>
</table>

Course offerings and teaching methods in academic year 2017-2018

A (semester 1) lecture 20.0 h

Lecturers in academic year 2017-2018

Bultinck, Patrick WE06 lecturer-in-charge

Offered in the following programmes in 2017-2018

<table>
<thead>
<tr>
<th>crdts</th>
<th>offering</th>
</tr>
</thead>
<tbody>
<tr>
<td>Master of Science in Chemistry</td>
<td>3 A</td>
</tr>
<tr>
<td>Exchange Programme in Chemistry (master's level)</td>
<td>3 A</td>
</tr>
</tbody>
</table>

Teaching languages

English

Keywords

Advanced quantum chemistry, Electron correlation, Density Functional theory, Reactivity

Position of the course

This course is a 2nd Master advanced quantum chemistry course, aiming at augmenting the students knowledge of advanced quantum chemistry so they are able to apply these methods independently and judge published results critically.

Contents

1. Hartree-Fock theory revisited
2. Electron correlation
3. Capita selecta of modern theories

Initial competences

Students must have acquired credit for quantum chemistry and Chemical Bond. Alternatively credits obtained for equivalent courses can be accepted where the equivalence is judged by the lecturer.

Final competences

1. Being able to judge the quality of published computational studies.
2. Being able to select the proper methods for a problem at hand.
3. Being able to apply quantum chemical techniques in a broader chemical environment.

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

Learning materials and price


(Approved)
References

Course content-related study coaching
Interactive support via the Minerva online system

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
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
During the course, students will have to write several reports and computer algorithms to show they master the subject. The union of all these reports are the basis for the final mark.

Calculation of the examination mark