

Computationele chemie (C002550)

Wegens Covid19 kan mogelijk afgeweken worden van de onderwijs- en evaluatievormen. Dergelijke afwijkingen zullen via Ufora worden gecommuniceerd.

Cursusomvang *(nominale waarden; effectieve waarden kunnen verschillen per opleiding)*

Studiepunten 6.0 **Studietijd** 170 u **Contacturen** 64.5 u

Aanbodsessies en werkvormen in academiejaar 2020-2021

A (semester 2)	Engels	Gent	werkcollege: PC- klasoefeningen	45.0 u
			hoorcollege	22.5 u

Lesgevers in academiejaar 2020-2021

Bultinck, Patrick	WE06	Verantwoordelijk lesgever
Acke, Guillaume	WE06	Medelesgever

Aangeboden in onderstaande opleidingen in 2020-2021

	stptn	aanbodssessie
Educatieve Master of Science in de wetenschappen en technologie (afstudeerrichting chemie)	6	A
Master of Science in Chemistry	6	A

Onderwijstalen

Engels

Trefwoorden

Computational chemistry, Molecular Modelling

Situering

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.

Inhoud

- 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

Begincompetenties

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.

Eindcompetenties

- 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.

Creditcontractvoorwaarde

Toelating tot dit opleidingsonderdeel via creditcontract is mogelijk mits gunstige beoordeling van de competenties

Examencontractvoorwaarde

Dit opleidingsonderdeel kan niet via examencontract gevolgd worden

Didactische werkvormen

Hoorcollege, werkcollege: PC-klasoefeningen

Toelichtingen bij de didactische werkvormen

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.

Leermateriaal

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.

Referenties

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

Vakinhoudelijke studiebegeleiding

Guidance by lecturer and assisting staff during computer classes and on appointment.

Evaluatiemomenten

periodegebonden en niet-periodegebonden evaluatie

Evaluatievormen bij periodegebonden evaluatie in de eerste examenperiode

Schriftelijk examen

Evaluatievormen bij periodegebonden evaluatie in de tweede examenperiode

Schriftelijk examen

Evaluatievormen bij niet-periodegebonden evaluatie

Verslag

Tweede examenkans in geval van niet-periodegebonden evaluatie

Niet van toepassing

Toelichtingen bij de evaluatievormen

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.

Eindscoreberekening

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.