

Computational Quantum Chemistry (C004148)

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 8.0 **Studietijd 210 u** **Contacturen** 115.0 u

Aanbodsessies en werkvormen in academiejaar 2020-2021

A (semester 2)	Engels	Gent	hoorcollege	15.0 u
			project	50.0 u
			werkcollege: PC- klasoefeningen	50.0 u

Lesgevers in academiejaar 2020-2021

Bultinck, Patrick	WE06	Verantwoordelijk lesgever
Acke, Guillaume	WE06	Medelesgever

Aangeboden in onderstaande opleidingen in 2020-2021

	stptn	aanbodsessie
Educatieve Master of Science in de wetenschappen en technologie (afstudeerrichting chemie)	8	A
Master of Science in Chemistry (afstudeerrichting Materials and Nano Chemistry)	8	A
Uitwisselingsprogramma chemie (niveau master)	8	A

Onderwijstalen

Engels

Trefwoorden

quantum chemical programming, software development, method development

Situering

This course follows up on a thorough introduction to molecular quantum mechanics and aims to familiarize the students with the implementation of quantum chemical methods, which are theoretically elaborated in the course 'Advanced Quantum Chemistry'. The emphasis in this course is on method development and not on molecular modeling.

Inhoud

- Modern software development: Linear algebraic software packages, Collaboration tools, Version control, Testing and code coverage, Continuous integration, Documentation, Building systems, Software design.
- Quantum Chemical Integrals: Obara-Saika, Libint.
- Hartree-Fock: RHF, UHF, DIIS.
- Perturbation theory on Hartree-Fock: MP2.
- Correlated Quantum Chemical Methods: CEPA0, CCD, CCSD, CIS, CISD, FCI.
- Response theory: CPHF, TDHF, CCLR.
- Orbital optimization.

Begincompetenties

An excellent training in quantum chemistry is required, amounting at least 12 ECTS credits in previous exposure to quantum chemistry, quantum mechanics and related fields. The course on Advanced Quantum Chemistry is most strongly recommended to be taken as well.

Eindcompetenties

- 1 The student obtains a highly advanced knowledge of modern quantum chemical methods.
- 2 The student is able to bring a theoretical method from the stage of model description

to an effective implementation.

- 3 The student is able to carry out large scale computational experiments on modern advanced computational infrastructure.
- 4 The student masters the area of software development in computational chemistry.

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, project, werkcollege: PC-klasoefeningen

Toelichtingen bij de didactische werkvormen

On campus lecture, online project and online tutorials with support through Ufora and MS Teams. Because of COVID19, changed working methods can be rolled out if this proves necessary.

Leermateriaal

An integrated course is offered via Ufora, where course notes and assignments from tutorials are supplemented with web lectures and knowledge clips. Each student must have their own computer with a webcam and microphone.

Referenties

- "Molecular Electronic-structure theory" T. Helgaker, P. Jorgensen & J. Olsen, Wiley, ISBN 0-471-96755-6

Vakinhoudelijke studiebegeleiding

Interactive support through Ufora 'Discussions'. Individual guidance by teachers / assistants: by electronic appointment via MS Teams.

Evaluatiemomenten

niet-periodegebonden evaluatie

Evaluatievormen bij periodegebonden evaluatie in de eerste examenperiode

Mondeling examen

Evaluatievormen bij periodegebonden evaluatie in de tweede examenperiode

Mondeling examen

Evaluatievormen bij niet-periodegebonden evaluatie

Werkstuk, verslag

Tweede examenkans in geval van niet-periodegebonden evaluatie

Niet van toepassing

Toelichtingen bij de evaluatievormen

- 1 The students gradually develop their own codes through first implementing methods of increasing complexity. Each implementation is separately marked and used as part of the non-periodic evaluation.
- 2 The final exam is the independent implementation of a quantum chemical method on a highly advanced computational infrastructure with focus on the efficiency of the program written in a modern programming language. After evaluation of the algorithm, the student is interviewed on the method and its implementation during an oral exam.

Eindscoreberekening

85% of the end score is based on the non-periodic evaluation. 25% is based on the evaluation of the reports for the implementation of methods during the seminars. 60% is based on the evaluation of the final and independent implementation of a method on a highly advanced computational infrastructure with focus on the efficiency of the program written in a modern programming language.

Failure to submit the reports within the deadline set, renders a zero score for each report.

The remaining 15% of the score is earned based on the oral exam on the implemented method and its implementation.