

## Computational Quantum Chemistry (C004148)

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

**Studiepunten 8.0** **Studietijd 210 u**

**Aanbodsessies en werkvormen in academiejaar 2023-2024**

A (semester 2)	Engels	Gent	hoorcollege werkcollege
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**Lesgevers in academiejaar 2023-2024**

Bultinck, Patrick	WE06	Verantwoordelijk lesgever
Acke, Guillaume	WE06	Medelesgever

**Aangeboden in onderstaande opleidingen in 2023-2024**

	stptn	aanbodsessie
<a href="#">Educatieve Master of Science in de wetenschappen en technologie (afstudeerrichting chemie)</a>	8	A
<a href="#">Master of Science in Chemistry (afstudeerrichting Materials and Nano Chemistry)</a>	8	A
<a href="#">Uitwisselingsprogramma chemie (niveau master)</a>	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 heavily relied on and is highly advised to be taken alongside this course..

**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**

Werkcollege, Hoorcollege

### **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**

Mondelinge evaluatie

### **Evaluatievormen bij periodegebonden evaluatie in de tweede examenperiode**

Mondelinge evaluatie

### **Evaluatievormen bij niet-periodegebonden evaluatie**

Werkstuk

### **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.