UNIVERSITEIT GENT

# Studiefiche

Academiejaar 2023-2024

## Advanced Quantum Chemistry (C004147)

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

**Studiepunten 4.0** **Studietijd 115 u**

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

| | | | |
|---|---|---|---|
| A (semester 2) | Engels | Gent | hoorcollege |
| | | | zelfstandig werk |

**Lesgevers in academiejaar 2023-2024**

| | | |
|---|---|---|
| Bultinck, Patrick | WE06 | Verantwoordelijk lesgever |
| Acke, Guillaume | WE06 | Medelesgever |

| Aangeboden in onderstaande opleidingen in 2023-2024 | stptn | aanbodsessie |
|---|---|---|
| Educatieve Master of Science in de wetenschappen en technologie(afstudeerrichting chemie) | 4 | A |
| Master of Science in Chemistry(afstudeerrichting Materials and Nano Chemistry) | 4 | A |
| Uitwisselingsprogramma chemie (niveau master) | 4 | A |

**Onderwijstalen**

Engels

**Trefwoorden**

electronic structure theory, electron correlation, ab initio methods

**Situering**

This course follows up on a thorough introduction to molecular quantum mechanics and aims to familiarize the students with modern electronic structure methods based on wave functions. This course provides the necessary theoretical background for the course 'Computational Quantum Chemistry'.

**Inhoud**

- Quantum chemical building blocks: Basis sets, Integrals, Spin
- Hartree-Fock theory: Self-consistent field, Roothaan-Hall, Pople-Nesbett
- Second quantization: Algebra of creation and annihilation operators, Wick's theorem, Kutzelnigg-Mukherjee and diagrammatic notation
- Modern electronic structure methods: Configuration interaction, Coupled cluster, Multiconfiguration self-consistent field, Many body perturbation theory
- Response theory: Molecular properties, Orbital relaxation

**Begincompetenties**

This course builds further on certain final competences of the courses:
- Mathematics: basic concepts
- Electronic structure
- Symmetry and spectroscopy

**Eindcompetenties**

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 develop new methdos independently.

**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, Zelfstandig werk

**Toelichtingen bij de didactische werkvormen**

De studenten krijgen gedurende de hoorcolleges de basisingedriënten van quantumchemische methoden aangereikt en vullen deze kennis verder aan via begeleide zelfstudie en flipped classroom.

**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: 978-1118531471
- "Many-Body Methods in Chemistry and Physics: MBPT and Coupled-Cluster Theory", I. Shavitt, R. J. Bartlett (Cambridge University Press), ISBN: 978-0521818322
- "Second Quantized Approach to Quantum Chemistry: An Elementary Introduction", P. R. Surjan (Springer Berlin Heidelberg), ISBN: 978-3642747571
- "Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory", A. Szabo, N. S. Ostlund (Dover Publications), ISBN: 978-0486691862

**Vakinhoudelijke studiebegeleiding**

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

**Evaluatiemomenten**

niet-periodegebonden evaluatie

**Evaluatievormen bij periodegebonden evaluatie in de eerste examenperiode**

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

**Evaluatievormen bij niet-periodegebonden evaluatie**

Werkstuk

**Tweede examenkans in geval van niet-periodegebonden evaluatie**

Examen in de tweede examenperiode is enkel mogelijk in gewijzigde vorm

**Toelichtingen bij de evaluatievormen**

The students write a report in which they critically approach a published method by means of a theoretical analysis that is detailed enough to start an implementation of that method.

**Eindscoreberekening**

Werkstuk: 100%