Module name	Theory
Number	2009-M03
Aims	Introduction into the most important quantum chemical methods for the study of the behavior of matter and the properties of molecules. Interpretation of the results of quantum chemical calculations. Application of quantum chemical methods to chemical problems.
Basics	(The topics are covered by lectures from existing master courses): Fundamentals of quantum chemistry: Interpretation of quantum mechanics, Schrödinger equation, approximation procedures in quantum chemistry
Contents	1. Introduction in theory: Hartree Fock method and density functional theory. 2. Potential energy surfaces, computational thermochemistry and theoretical spectroscopy. 3. Practical course: Introduction in computational chemistry: Handling of modern quantum-chemical programs (Turbomole). Applications of quantum chemical methods to chemical problems.
Methods	Hartree-Fock and density functional theory (DFT)
Type	Two-day block course/ June 30, July 1
Work load	15 hours presence/ 45 hours self-study
Examination	oral/ written
Credit points	2
Responsible scientists	Kirchner
International guest lecturers	Reckien
Industrial partners	
Recommendations for literature, e-learning	F. Jensen, *Introduction to Computational Chemistry* (Wiley & sons, 2007) A. Szabo, N. S. Ostlund, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, Dover Pubn Inc (1996) I. N. Levine, *Quantum Chemistry,* Prentice Hall (2008) F. L. Pilar, *Elementary Quantum Chemistry,* Dover Pubn Inc (2001) P. W. Atkins, R. S. Friedman, *Molecular Quantum Mechanics, (*Oxford University Press, 1999)

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SCHEDULE

Time	Lecturer	Program	Location
Day 1,			
9-11	Kirchner	Lecture: Introduction in Quantum Chemistry Part I: Hartree-Fock Theory	Johannis-allee 29 SR 102
11-13	Kirchner	Lecture: Introduction in Quantum Chemistry Part II: Hartree-Fock Theory	Johannis-allee 29 SR 102
14-15	Reckien/Kirchner	Lecture/Presentation: Introduction in Computational Chemistry	ThC
15-18	Reckien/Kirchner	Practical exercises in Computational Chemistry	ThC
Day 2,			
9-11	Reckien	Lecture: Introduction in Quantum Chemistry Part III: Density Functional Theory	Johannis-allee 29 SR 115
11-13	Reckien	Lecture: Introduction in Quantum Chemistry Part IV: Post Hartree-Fock Methods	Johannis-allee 29 SR 115
14-17	Reckien/Kirchner	Practical exercises in Computational Chemistry	ThC
17-18	Reckien/Kirchner	Presentation and discussion of the results of the practical exercises	ThC

Location: ThC: Chair of Theoretical Chemistry (Neubau)

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