MNF-chem1004D	Theoretical Chemistry / Computational Chemistry		
Semester / Duration	Annually: winter or summer term Duration: 2 Semesters		
Responsible faculty	Prof. Dr. Bernd Hartke, phone: 0431-880-2753, Email: hartke@pctc.uni-kiel.de Prof. Dr. Dassia Egorova, phone: 0431-880-7741, Email : egorova@phc.uni-kiel.de		
Degree programme	M.Sc. Chemie: 1. – 3. Fachsemester M.Sc. Physik: 1. – 3. Fachsemester M.Sc. in Business Chemistry: 1. – 2. Fachsemester M.Sc. Biochemistry and Molecular Biology: 1. – 3. Fachsemester		Compulsory elective (Wahlpflicht)
Questions and consultation	Prof. Dr. Bernd Hartke, phone: 0431-880-2753, Email: hartke@pctc.uni-kiel.de Prof. Dr. Dassia Egorova, phone: 0431-880-7741, Email : egorova@phc.uni-kiel.de		
Classes	**Name of Class / Lecturer**	**SWS**	**Status**
	Lectures on Theoretical Chemistry by Prof. Hartke, summer term only	2 SWS	compulsory
	Lecture and tutorials on Quantum Mechanics and Quantum Dynamics by Prof. Egorova	2 SWS	compulsory
	Lectures on Molecular Modelling by Prof. Herges, winter term only	2 SWS	compulsory
	Practical part by Prof. Hartke	3 SWS	compulsory
	Practical part “Quantum dynamics with MCTDH” by Prof. Egorova	3 SWS	compulsory
	Practical part by Prof. Herges	2 SWS	compulsory
Number of participants	15		
Language	German or English (as needed)		
Work Load	Classes: 200 h Self study: 250 h		
Credit Points	15		
Conditions	B.Sc. in Chemistry/Business Chemistry/Biochemistry/Physics or related discipline		
Prerequisites (desired and recommended)	Basic lnowledge on clasical and quantum mechanics, MNF-chem0304, MNF-chem0503		
Goals	Extension of knowledge in areas of molecular mechanics, quantum chemistry and quantum dynamics; development of capabilities to apply this knowledge as well as modern computational methods to particular problems of master and PhD projects.		
Contents	• Classical methods of molecular mechanics and molecular dynamics (force fields, MD, thermodynamics, Monte Carlo), • Quantum mechanics: formalism and exactly solvable problems; approximate methods (perturbation theory, variational principle); many-particle systems; diatomic systems; Basic principles of quantum chemistry (Hartree-Fock), • Quantum chemistry: SCF, DFT, electron correlation (CI, CC, MP2, MCSCF/CASSCF), • Quantum dynamics: Born-Oppenheimer, potential surfaces, wave packets, densitymatrix methods, MCTDH, • Practical part: force-filed and MD simulations, development of own computer codes,MCTDH, • Seminar talks.		
Key Qualifications	• Understanding of basic principles of force-fields and ab initio methods as well as of quantum dynamics. • Ability to select and apply the methods to particular problems; ability to analyse the obtained results. Application of methods for rational design of experiments		

	and drugs
Exam(s)	Examination forms: • Written or oral exam (Egorova), • practical part performance (Hartke, Herges), • written summary practical part (Egorova), • Seminar presentation (Hartke).
	Exams take place once each course is competed.
	Examination lanquage: German or English
	Final course grade is relevant for the M.Sc. Grade. It is calculated as an average over all examination forms listed above.
Literature	• Szabo/Ostlund, Modern Quantum Chemistry, McGraw-Hill, • Simons/Nichols, Quantum Mechanics in Chemistry, Oxford, • F. Jensen, Introduction to Computational Chemistry, Wiley, • D. J. Tannor, An Introduction to Quantum Mechanics – a Time-dependent Perspective, University Science Books, • R. Leach, Molecular Modelling, Prentice Hall, • P.W. Atkins, Molecular Quantum Mechanics, • I.N. Levine, Quantum Chemistry, • A.S. Davydov, Quantum Mechanics (Quantenmechanik), • G.C. Schatz, M.A. Rantner, Quantum Mechanics in Chemistry, • H.-D. Meyer, F. Gatti, and G. A. Worth (ed.), Multidimensional Quantum Dynamics: MCTDH Theory and Applications.
Comments & Notes	The practical part consists of 3 subunits (Hartke, Egorova, Herges). It may take place in summer or winter term or as a compact course during a semester break. Unit Hartke may be completed anytime. For units Egorova and Herges it is recommended to complete the practical part after having followed lectures and tutorials.