Module Name						
Advanced Theoretical Chemistry 1						

Type of Module			Module Code			
Basic Module			BM-C-TC1			

Identification Number	Workload	Credit Points	Term	Offered Every	Start	Duration
MN-C-A-TC1	180 h	6 CP	Winter semester	WiSe	Winter Term Only	1 Semester

1	Course Types	Contact Time	Private Study	Planned Group Size
	a) Lecture b) Exercise	45 h 15 h	60 h 60 h	<20 Students

2	Module Objectives and Skills to be Acquired
	Linear Algebra, Approximations, Quantum Mechanics, Many-Particle Systems

3	Module Content

	- Quantum mechanics I:
	    - experiments spin sorting machine, double slit
	    - fail of classical physics
	- Linear algebra
	    - group, field, linear space, scalar product, function space
	    - (vector) representations, approximations, Fourier transformation
	    - operators, operator representations
	    - eigen basis, eigenfunction approximation, variance
	    - matrices and operators
	    - linear transformations: mirror, rotation, scale, shere, SO(3), O(3)
	- Quantum mechanics II: mathematical description
	    - postulates, time propagation (Schrödinger equation)
	    - measurement projection, eigenfunction expansion, expectation value
	    - spin, SU(2)
	- Many body systems
	    - particle types, product ansatz, anti-symmetry
	    - configuration interaction (CI), Hartree-Fock (HF)
	    - 1- and 2-density(matrices)
	    - density functional theory

4	Teaching Methods
	Lectures and tutorials. Compulsory attendance in tutorials.

5	Prerequisites (for the Module)
	Formally: none With regard to contents: Basic Math Skills, Quantum Mechanics Basics

6	**Type of Examination** written exam, alternatively: oral
7	**Credits Awarded** The module is passed by passing the exam at the end of the module
8	**Compatibility with other Curricula** The module is part of the Master of Science in Chemistry
9	**Proportion of Final Grade** 6/114
10	**Module Coordinator** M. Hanrath
11	**Further Information** teaching language: English