Module Name
Advanced Theoretical Chemistry 2

Type of Module	**Module Code**
Basic Module	BM-C-TC2

Identification Number	**Workload**	**Credit Points**	**Term**	**Offered Every**	**Start**	**Duration**
MN-C-A-TC2	180 h	6 CP	Summer semester	SuSe	Summer 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

2nd Quantization, Feynman Diagrams, Coupled Cluster

3 Module Content

- Introduction
  - many-body wavefunctions
  - information carried by determinant
- 2nd quantization I: basic principles, idea
  - minimal representation: occupation number vectors
  - creators and annihilators: anti-commutation relations
  - function spanning and physical operators
  - size consistency: CI vs. coupled cluster (CC) ansatz
  - operator ranks
- 2nd quantization II: calculus
  - normal order
  - contractions
  - Wick's theorem (I) and (II)
  - particle/hole formalism
  - CC equations
- Feynman, Goldstone, Hugenholz diagrams
  - motivation, information, redundance, irrelevance
  - translation Algebra ↔ Diagram
  - elimination of remaining redundant information
  - Hamilton and cluster operators in diagrammatic form
  - contractions and CC equations in diagrammatic form

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, having attended “Advanced Theoretical Chemistry (Winter)”
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