

Announcement of the Lecture 21355 V/Ü (2+2):

**Quantum Chemistry on the Computer I (old master)  
Quantum Chemical Correlation Methods (new master)**

Lectures: Tuesday, from 06.05.2014 on, 16-18h, SR 36.07 (Takustr. 3)

Tutorials: Monday, from 05.05.2014 on, 12-14h, CIP-Pool Library, (Takustr. 3)

Exception: First lecture: Friday, 25.04.2014, 10-12h, SR 23.01 (Takustr. 3)

Content of the lecture and the tutorials:

Short repetition on Hartree-Fock-Roothaan-Hall method

Second quantization formalism

Wavefunction-based correlation method

- Configuration interaction
- Coupled cluster method
- Perturbation theory
- Multi-configurational SCF
- Multi-reference methods (both CI and perturbative approaches)

Quantum chemical description of excited states

Application of the above mentioned methods with the quantum chemical program MOLPRO including symmetry

- Prerequisite: Quantum Chemistry
- There will be computer exercises which must be solved and are marked. There will be an individual project for each student, which has to be solved and presented in a short talk at the end of the term.
- Tutor: Dr. Doreen Mollenhauer (Room 35.18)