
Winter Term 2018/2019

Announcement of a lecture (21341a, 2 hrs / week) with tutorials (21341b, 2 hrs / week)

Quantum Chemistry on the Computer I: Correlation Methods

Topics include:

- Hartree-Fock (short repetition)
- Second Quantization
- Configuration Interaction (CI)
- Coupled Cluster (CC)
- Perturbation Theory
- Multi-Configuration SCF
- Multi-Reference Methods
- Excited States

Tutorials:

- Method applications (software: MOLPRO, ...)

Dates & Times:

Lecture: every Tuesday, 16:00 – 18:00, SR 24.16, Takustr. 3, starting on 16.10.2018

Tutorials: to be arranged in the first lecture

- **Prerequisite:** Quantum Chemistry (LV 21311)
- **Note:** This course will take place only if at least 5 students enroll.
- Tutorials consist of computer exercises, which must be solved and which are marked. In addition, each student chooses an individual project, to be worked on during the term, and gives a short presentation (15 min) of her/his results at the end of the lecturing period (mid of February 2019).

For more information see <https://userpage.fu-berlin.de/~dandrae>