Freie Universität Berlin

Institut für Chemie und Biochemie
Prof. Beate Paulus
☎ (030) 838 52097
E-Mail: b.paulus@fu-berlin.de

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

Quantum Chemistry on the Computer I: Correlation Methods

Lecture: Tuesday, 16-18, SR 36.07 (Takustr. 3), start 14.04.2015
Tutorials: Time will be arranged in the first lecture

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 approached)

Quantum chemical descriptionn of excited states
Application of the above metioned methods with the quantum chemical program Molpro

- 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: Edoardo Fertitta (Room 35.20)
- The course will only take place if at least 5 students attend the course