Freie Universität Berlin

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Announcement of the Lecture 21358 V/Ü (2+3):

Quantum Chemistry on the Computer I

Preliminary Meeting: Tuesday, 12.04.2011 12.15 h, SR 24.16 (Takustr. 3)

Content of the lecture and the tutorials:

Introduction to the program codes GAUSSIAN, TURBOMOLE and MOLPRO

Basis sets and effective core potentials, basis set superposition error and counterpoise correction

Molecular symmetry in quantum chemical calculations

Hartree-Fock approximation, convergence criteria for the self-consitent field procedure

Localization of orbitals

Single-reference correlation methods (configuration interaction, perturbation theory, coupled cluster)

Calculation of properties and expectation values

Optimization of molecular structure, potential energy surfaces and vibrational frequencies

Multi-reference methods and excited states

- There will be computer exercises which must be solved and handed in in written form for marking. Additionally, each participant has to solve an individual problem and present the results orally and in written form.
- Tutors (depending on the topic): Dr. Carsten Müller (Room 35.18), PD Dr. Dirk Andrae (Room 35.14), Dr. Elena Voloshina: (Room 35.14).
- Further informations on the homepage AG Paulus under „Teaching“ or directly from Prof. Beate Paulus (Room 35.17).
- In the second part (WS 11/12) the topics will focus on the density functional methods.