Freie Universität Berlin

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

Quantum Chemistry on the Computer II

Preliminary Meeting: Monday, 17.10.2011 12.15 h, SR 24.16 (Takustr. 3)

Content of the lecture and the tutorials:

Introduction to computational chemistry
The use of different quantum chemical programs
GAUSSIAN, TURBOMOLE and MOLPRO
Density functional theory and different functionals
Treatment of excited states
Calculation of molecular properties
Multi-reference correlation methods

- Prerequisite: Quantum Chemistry, but not Quantum Chemistry on the Computer I,
- There will be computer exercises which must be solved and handed in in written form for marking.
- Tutor: Dr. Carsten Müller (Room 35.18)
- Further informations directly from Prof. Beate Paulus (Room 35.17).