

Ankündigung der Vorlesung 21311 V/Ü (2+2):

Quantum chemistry
in English

Lecture:	Monday 10-12, Arnimallee 22, Hörsaal A Start 11.04.2011
Tutorials:	Wednesday 12-14, Takustr. 3, 34.16/17 Start 13.04.2011, Tutor Lukas Hammerschmidt
Exam - Part 1	Wednesday, 01.06.2011, 12-14
Exam - Part 2	Wednesday, 20.07.2011, 10-12
Retake Exam - Part 1 and 2	Monday, 19.09.2011, 10-14

Content of the lecture:

Basics of quantum theory and simple systems (angular momentum, H-atom, spin)
Born-Oppenheimer approximation and potential energy surfaces for chemical reactions
Hartree-Fock approximation, LCAO-MO approximation and basis sets
Approximations of the integrals and semi-empirical methods (e.g. Hückel theory)
Correlation methods (configuration interaction, perturbation theory)
Density-functional methods
Special topics

- There will be one exercise per week as homework. 75% of the homeworks must be solved fully and handed in to the tutor in written form.
- Further informations on the homepage AG Paulus under „Teaching“ or directly from Prof. Beate Paulus (Room 35.17, email: b.paulus@fu-berlin.de).