

Announcement of the Course 21311 a/b (2+2):

Quantum chemistry (in English)

Lecture:	Monday 10-12, Takustr. 6, Hörsaal Start 13.10.2014
Tutorials:	Monday 12-14 Wednesday 12-14
Exam - Part 1	8.12.2014, 10-12, Hörsaal A, Henry-Ford-Bau
Exam - Part 2	23.2.2015, 10-12, Hörsaal 2, Silberlaube
Retake Exam - Part 1 and 2	26.3.2015, 8-12, Königin-Luise-Str. 12-16a Großer Hörsaal

Content of the lecture:

Basics of quantum theory and simple systems
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
Molecular properties

Additional informations:

- Within the tutorials both analytic and computational exercises will be offered.
- This course will be suitable both for the new and the old master study in chemistry.
- Further informations on the homepage AG Paulus under „Teaching“ or directly from Prof. Beate Paulus (Room 35.15, email: b.paulus@fu-berlin.de).