

Announcement of the Course 21321 a/b (2+2):

Quantum chemistry (in English)

Lecture:	Monday 10-12, Takustr. 6, Hörsaal Start 12.10.2015
Tutorials:	Monday 12-14 Wednesday 12-14 Start 19.10.2015 and 21.10.2015
Exam - Part 1	Mid of December, to be announced
Exam - Part 2	Mid of February, to be announced
Retake Exam - Part 1 and 2	End of March, to be announced

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.
- The lecture will be given together with Dr. Jhon Fredy Perez-Torres
- Further informations on the homepage AG Paulus under „Teaching“ or directly from Prof. Beate Paulus (Room 35.15, email: b.paulus@fu-berlin.de).