

Announcement of the Lecture 21311 V/Ü (2+2):

## Quantum Chemistry

Lecture	Monday 8h, SR 36.07, Takustr. 3, start 20.04.2009
Tutorials	Monday 10h, SR 26.07 (A-M) and SR 36.07 (N-Z)
Exam - Part 1	Monday, 08.06.09, 8 - 10
Exam - Part 2	Monday, 20.07.09, 10 -12
Repetition of the Exam	Monday, 21.09.09, 10 - 14 (Two parts)

Content of the Lecture:

Basics of quantum theory and simple systems (angular momentum, H-atom, spin)  
Born-Oppenheimer approximation and potential energy surface 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 and handed to the tutors in written form.
- Tutors:
  - Dr. Elena Voloshina: Room 35.14
  - Doreen Mollenhauer: Room 35.18
- Further informations on the homepage AG Paulus under „Teaching“ or directly from Prof. Beate Paulus (Room 35.17).