

**Atomic and molecular physics**  
**themes of the comprehensive exam**

1. Eigenvalue problem of the attractive Coulomb potential: the primary spectrum of the Hydrogen atom, the fine structure and other corrections
2. Stark effect and polarizability of the H atom
3. Spin and orbital angular momentum, addition of angular momenta
4. The spectrum of the He atom: ground state and excited states with perturbation theory, singlet and triplet states, exchange interaction
5. The variational method and its application for the ground state of the He atom
6. The one-electron approximation for atoms, the Hartree and Hartree-Fock methods
7. Electronic configurations of atoms, spin-orbit couplings, Hund's rules.
8. Selection rules and atomic spectra.
9. Atoms in magnetic fields, Zeeman effect
10. The eigenvalue problem for molecules, separation of nuclear and electronic motion, adiabatic and Born-Oppenheimer approximations
11. Molecular orbitals for the  $H_2^+$  molecular ion and the  $H_2$  molecule, the VB method
12. The Hartree-Fock method for molecules, the Roothaan equations.
13. The origin of the chemical bond, the virial theorem
14. Rotational spectra of diatomic molecules, centrifugal distortion
15. Vibrational spectra of diatomic molecules, harmonic and anharmonic oscillations, vibrational transitions.
16. Electronic states of multielectron atoms, hybridization, simple molecules:  $H_2O$ ,  $CO_2$ ,  $NH_3$
17. Spectra of multiatomic molecules, electronic transitions, vibrational and rotational structure, fluorescence and Raman spectra.

Literature:

- W. Demtröder: Atoms, Molecules and Photons, Springer, 2006  
B. Bransden, C. Joachain: Physics of Atoms and Molecules, 2nd ed, Prentice Hall 2003  
P. Atkins, R. Friedman: Molecular quantum mechanics 4th ed., Oxford 2005