

## **Quantum chemistry – 0351-3212 – Syllabus**

- ✓ Mathematical introduction.
- ✓ Problem definition.
- ✓ The Born-Oppenheimer approximation: definition of the electronic Hamiltonian.
- ✓ Hartree and Hartree-Fock approximations.
- ✓ Gaussian basis set representations.
- ✓ Roothan equations - the algebraic form.
- ✓ Hohenberg-Kohn density functional theory.
- ✓ The Kohn-Sham scheme.
- ✓ Exchange-correlation density functional approximations.