1. Postulates of quantum mechanics; formalism and interpretation of quantum mechanics.
2. One-dimensional and multi-dimensional model systems: particle in a box, potential barriers, harmonic oscillator, rigid rotator; hydrogen-like atom.
3. Multielectron atoms: periodic table of elements, total quantum numbers and atomic terms (weak coupling).
4. Principles of approximate computational methods of quantum chemistry: variational method; Born-Oppenheimer approximation, one-electron approximation, Hartree-Fock method, LCAO MO method and its analytical formulation, sources of errors in the HF method, ab initio methods and semi-empirical methods.
5. Fundamentals of density functionals theory: electron density and the wavefunction; Hohenberg-Kohn theorem, Kohn-Sham method, exchange-correlation functionals.
6. Post-HF methods (the concept of configuration, Slater-Condon rules, MP perturbation theory, CI method, MC SCF method, Brillouin's theorem, variants of CI and MP methods, size consistency).
7. Accuracy of the computational-methods of quantum chemistry.
8. Fundamentals of quantum-chemical molecular modelling: potential energy hypersurface and stationary points, optimization of geometry of molecular systems, electronic structure description, molecular orbitals versus localized orbitals, population analysis and bond multiplicity indexes, vibrational analysis, optimization of transition state geometry, modelling of chemical reactivity - kinetics and thermodynamics of reactions; reactivity indices - molecular electrostatic potential, frontier orbitals theory and Fukui functions.
9. Elements of statistical thermodynamics: basic thermodynamic potentials, principles of phenomenological thermodynamics, entropy as a link between the micro and macroworld, phase space μ and μ, Liouville equation, basic statistical ensembles, partition function, ideal gas, statistical description of the basic states of matter (real gas, liquid and solid state), simulation methods.
10. Spectroscopy: molecular symmetry, selection rules, rotational and vibrational spectra, normal vibrations, IR and Raman spectra, anharmonicity, electronic spectra, vibrational structure, electronically excited states, absorption and emission spectra, laser action.
11. Electrical and magnetic properties of molecules, dipole moments, polarizability and induced dipole moments, intermolecular interactions.

Literature (in English):

L. Piela, "*Ideas of Quantum Chemistry*", Elsevier

J. de Paula, P. Atkins, *"Physical Chemistry",* Oxford University Press

F. Jensen, "*Introduction to Computational Chemistry"*, Wiley