Quantum theory of molecules and polymers (KDIT34)

topics

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1. **Elements of quantum mechanical description:**
   - State, measurable quantities, measurements, time evolution.
   - Operators of molecular systems. Schrödinger's equation of atoms and molecules. Atomic units.
   - Identical particles. The symmetrization postulate.
   - Fundamental methods of approximation I: Calculus of variations (functional, functional derivative, variation of functionals).
   - Fundamental methods of approximation II: Perturbation calculus (non-degenerate, time-independent Rayleigh-Schödinger perturbation theory).
   - Time-dependent perturbation calculus, selection rules.
   - Formalism of second quantization.
2. **Quantum mechanical description of molecules**
   - Separation of electronic and nuclear motions. Born-Oppenheimer approximation, adiabatic approximation.
   - Molecular vibrations, IR spectrum, molecular symmetry.
   - Solution of the Schrödinger equation by separation. The independent particle model. Pauli principle.
   - Hartree-Fock method. Single particle states, orbits. Koopmans theorem.
   - Open and closed shell systems. RHF and UHF equations.
   - Hartree-Fock-Roothaan-Hall equation.
   - Electron correlation. Many-body perturbation theory.
   - Configuration interaction (CI), coupled cluster (CC) method.
   - Multiconfiguration-SCF (MC-SCF), complete active space-SCF (CAS-SCF).
   - Calculation of excited states by the EOM method.
   - Reduced density matrices.
   - Hohenberg-Kohn theorems.
   - Kohn-Sham equation. Exchance-correlation potentials.
   - Time-dependent density functional theory (TDDFT): Runge-Gross theorem, van Leeuwen theorem.
   - Time-dependent Kohn-Sham equation.
3. **Periodic polymers, solid-state physics model**
   - Quantum mechanical description of quasi 1D periodic systems
   - The role of symmetry, Bloch's theorem
   - Basics of band theory. Applications.