

Basic Ideas of Quantum Chemistry

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1. Postulates of quantum mechanics
2. The Schrödinger equation and its exact solutions: particle in a box, harmonic oscillator, rigid rotator, hydrogen atom
3. Variational method
4. Born-Oppenheimer approximation: “molecular structure”, foundations of the electronic, vibrational and rotational spectroscopy.
5. Motion of the nuclei: normal modes, force fields, molecular mechanics, molecular dynamics
6. Molecular orbitals (Hartree-Fock method, Self-Consistent Field, LCAO approximation, localization of orbitals)
7. Beyond the Hartree-Fock approximation (Configuration Interaction, Density Functional Theory)

Termin	Dzień tygodnia	Godzina	Miejsce
03.06.2013	Poniedziałek	12.15 – 15.00	Minicentrum Konferencyjne (Luwr)
04.06.2013	Wtorek	12.15 – 15.00	Minicentrum Konferencyjne (Luwr)
05.06.2013	Środa	12.15 – 15.00	Minicentrum Konferencyjne (Luwr)
06.06.2013	Czwartek	12.15 – 15.00	Minicentrum Konferencyjne (Luwr)
07.06.2013	Piątek	12.15 – 15.00	Minicentrum Konferencyjne (Luwr)