ITMO University

Methods of Quantum Chemistry

Course Workload		Assessment form (examination/ graded test/ ungraded test)
ECTS	Hours	
6	216	Exam

The course contains the basic concept and general methods of quantum-mechanical modeling of nanosystems. Practical lessons are devoted to the application of modern software packages, such as “PC GAMESS”, “GAUSSIAN”, “HYPER CHEM”, “QUANTUM-ESPRESSO”, “GPAW”, “MOPACK”, “MERCURY” to modeling of the optimum geometry, electronic structure and optical response of periodic and non-periodic systems.

Course structure:

1. Introduction

1.1. Basics of quantum many bode theory (Hartree-Fock approximation and the density functional theory)

2. Modeling of molecular systems

2.1. The Hukel molecular orbital theory, Born-Oppenheimer approximation, valence bond method, molecular orbital method

3. Realization of density functional theory for computation of optimal geometry and electronic structures of atomic and molecular systems

3.1. Realization of density functional theory for computation of optimal geometry and electronic structures of atomic and molecular systems

3.2. The calculation of optimized geometry and electronic structure of atomic and molecular systems with use of atomic orbitals basis set – application of FireFly quantummechanical modeling package

4. Realization of density functional theory for computation of optimal geometry

4.1. Realization of density functional theory for computation of optimal geometry, electronic structures, density of states and band structure of periodic systems with use of plane wave basis set
4.2. The calculation of optimal geometry, electronic structures, density of states and band structure of periodic systems with use of plane wave basis set – application of QUANTUM ESPRESSO quantum-mechanical modeling package with use of GUI BURAI
4.3. The calculation of optimal geometry, electronic structures, density of states and band structure of periodic systems with use of plane wave basis set – application of QUANTUM ESPRESSO quantum-mechanical modeling package with use GUI QUANTUM VITAS.

5. The time-dependent density functional theory and their application to calculation of optical response of periodic and non-periodic systems

5.1. The time-dependent density functional theory and their application to calculation of optical response of periodic and non-periodic systems.
5.2. The calculation of optical response of periodic systems – application QUANTUM ESPRESSO quantum-mechanical modeling package with use GUI QUANTUM VITAS

6. The two-particle Green's function

6.1. The two-particle Green's function. The two-particle vertex. Hedin's equations. GW approximation. Bethe-Salpeter equation
6.2. Realization of GW approach for periodic systems – application QUANTUM ESPRESSO quantum-mechanical modeling package