**Name of the course**: “Quantum Chemistry”

**Department responsible for the course or equivalent:** Dpt of Chemistry

**Lecturer (name, academic title, e-mail**): Dr. I.N.Shcherbakov,

[shcherbakov@sfedu.ru](mailto:shcherbakov@sfedu.ru)

**Semester when the course unit is delivered: 1**

**Teaching hours per week:** 4

**Level of course unit:** Master level.

**ECTS credits: 5**

**Admission requirements:** Course “Computational Chemistry” require the basic knowledge of the quantum theory, electronic structure of the atoms and molecules along with the bachelor’s level knowledge selected fields of mathematics, general physics and general chemistry.

Course “Computational Chemistry” is mandatory for studying courses “Advanced Chemistry of the Elements”, “The theory, structure and magneto-chemistry of coordination compounds”.

**Course objectives (aims):** The course is developed to feel the gap between the basic knowledge of quantum chemistry and practical planning, implementation and results interpretation of computational study aimed on the modeling of the structure and physical-chemical properties of the molecular substances. The most widely used concepts and approximations are being discussed from the aspect of the quantum-chemical modeling and utilization of the most popular quantum chemical packages is covered in the practical course (Gaussian, GAMESS and ORCA).

Fields covered are *ab initio*, density functional theory (DFT), semiempirical and molecular dynamics approaches, modelling of the excited states and spectroscopic properties, study of the mechanism and evaluation of kinetic parameters of the chemical reactions.

**Course contents:** Scope of computational chemistry. Overview of programs. Parallel computing. Mainstream modelling tools. Molecular mechanics. Quantum chemistry methods hierarchy. Semiempirical methods. *Ab initio* methods. Introduction to electron correlation. Configuration interaction. Many-body perturbation theory. Coupled-cluster theory. Density functional theory. Excited electronic states modelling. Spectral properties evaluation.

Basis sets. Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets, correlation-consistent sets. Basis set superposition error (BSSE). Effective core potentials (ECP).

Electronic distribution analyses tools – Mulliken charge distribution, AIM (Bader) analysis, NBO. Graphical tools for structure and electronic distribution visualization.

The PES concept. Geometry optimization. Transition states search. Vibrational frequency analysis. Thermodynamics and kinetic of the chemical reactions. Molecular dynamics.

The solvation process and the incorporation of its effects in molecular modelling. Implicit and explicit solvate accounting methods.

**Planned learning activities and teaching methods –** lectures with a variety of examples and practice.

**Assessment methods and criteria:** examination