ITMO University

Computational Chemistry and Modeling of Chemical Systems

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

Since theoretical data are inextricably linked with experimental data and are potentially capable of enhancing the performance and interpretability of predictive machine learning algorithms, students will be trained in modeling chemical systems, as well as theoretical calculations of their properties, and gain an understanding of how experimental data can be enhanced by the results obtained in the context of individual chemical tasks. The course is aimed at teaching High-throughput DFT calculation, molecular docking of pharmaceuticals to targets. Students will understand the methods of molecular modeling, quantum chemical calculations, molecular docking, density functional theory (DFT); principles of model construction, optimization of molecular geometry; be aware of the limitations and applicability of methods for solving chemical problems; the concept of "multiphysical modeling of complex systems". Students will be able to analyze the work of the constructed models, interpret from the point of view of chemistry and materials science, visualize and present the results obtained. Students will have the skill of using packages and libraries for calculations and database constructions for further analysis by machine learning methods.

Course structure:

1. Introduction to computational chemistry

1.1. Describing the system
1.2. Fundamental forces
1.3. The dynamical equation
1.4. Classical mechanics
1.5. Quantum mechanics

2. Force field methods

2.1. The force field energy: 2.1.1. Stretch energy 2.1.2. Bending and out-of-plane bending energy 2.1.3. Torsional energy 2.1.4. van der Waals energy 2.1.5. Electrostatic energy
2.2. Force field parameterization

2.3. Atomistic force fields
2.4. Coarse grained force fields
2.5. Transition structure modeling

3. Hartree-Fock theory

3.1. Adiabatic and Born-Oppenheimer approximations
3.2. HF theory
3.3. Slater determinant energy
3.4. Koopmans’ theorem
3.5. The basis set approximation
3.6. Self-consistent field (SCF) techniques
3.7. Periodic systems

4. Electron correlation methods

4.1. Excited Slater determinants
4.2. Configuration interaction
4.3. Multiconfiguration SCF
4.4. Many-body perturbation theory
4.5. Coupled cluster
4.6. Interelectronic distance
4.7. Quantum Monte Carlo methods

5. Basis sets

5.1. Slater- and Gaussian-type orbitals
5.2. Classification of basis sets
5.3. Construction of basis sets
5.4. Standard basis sets
5.5. Plane wave basis functions
5.6. Grid and wavelet basis sets
5.7. Fitting basis sets
5.8. Effective core potentials

6. Density functional methods

6.1. Orbital-Free Density Functional Theory
6.2. Kohn-Sham theory
6.3. Reduced Density Matrix and Density Cumulant Methods
6.4. Exchange-correlation functionals
6.5. Ensemble DFT

7. Overview of other methods

7.1. Semi-empirical methods: 7.1.1. Assumptions to differential overlap 7.1.2. Parametrization 7.1.3. Huckel theory 7.1.4. Tight-binding DFT
7.2. Valence bonds methods: 7.2.1. Classical valence bond theory 7.2.2. Spin-coupled valence bond theory 7.2.3. Generalized valence bond theory
7.3. Relativistic methods: 7.3.1. Dirac equation 7.3.2. Connections between Dirac and Schrodinger equations 7.3.3. Many-particle systems

8. Other properties derived from Schrodinger equation

8.1. Wave function analysis
8.2. Molecular properties
8.3. Illustrating the concepts
8.4. Optimization techniques

8.5. Statistical mechanics
8.6. Simulation techniques
8.7. Qualitative theories
8.8. Mathematical methods
8.9. Statistics and QSAR