Study program : Chemistry

Type and level of studies: PhD studies

Course unit: Molecular modeling in inorganic chemistry

Teacher in charge : Matović D. Zoran

Language of instruction: English

ECTS: 10

Prerequisites: Passed compulsory courses

Semester: *Summer Semester*

Course unit objective

Educate students in the field of computer chemistry with the acquisition of knowledge of basic molecular mechanics and quantum mechanics (ab initio and DFT) while working with the most software packages: Gausian, Spartan, ADF, Hiperchem.

Learning outcomes of Course unit

The student should acquire knowledge of the basics of modeling, which includes the ability to create and manipulate three-dimensional molecular files with various formats (mol, PDB, XYZ, ent, mol2, hin, CIF) using available software packages. Also, the student should acquire knowledge in order that these molecular structures further processed and analyzed using molecular mechanics (optimization of geometry, conformational search) and quantum mechanics - HF and DFT methods (geometry optimization, calculation of vibrational frequencies, excitation conditions, transients, etc.). The student should know what are the advantages and disadvantages of what molecular mechanics in relation to quantum mechanics and to successfully take advantage of the combined method of molecular mechanics and quantum mechanics. All this should serve the student to modeling and simulation predict the physical chemical conditions (reaction mechanisms, IR and UV spectra, NMR and EPR spectra) molecules of interest.

Course unit contents

Fundamentals of computer chemistry; Modeling of molecular mechanics; Modeling of quantum mechanics; Density functional theory (DGT); Examples of modeling coordination compounds DFT software packages - ADF and Gausian; Options in computer modeling; Unit point on the surface of potential energy; local minimum on the surface of potential energy; Transitional structures on the surface of potential energy; Molecular dynamics on the surface of potential energy; UV-visible spectroscopy; Vibration analysis and IR spectroscopy

Literature

1. F. Weinhold and C. R. Landis, *Valency and Bonding*

Number of active teaching hours				**Other classes /**
Lectures: 5	Practice: /	Other forms of classes:/	Independent work: /	

Teaching methods All aspects of contemporary teaching (graphics, audio and video) in modern auditoriums with video beam, projector and blackboard; Methods of Exercise: Practical classes will be conducted in computer labs where students will be able to independently perform kompjutacione experiments under the supervision of teachers.

Examination methods (maximum 100 points)

Exam prerequisites	**No. of points:**	**Final exam**	**No. of points:**
Student's activity during lectures	/	oral examination	25
practical classes/tests	20	written examination	25
Seminars/homework	30	.....	
Colloquiums	/		
Other	/		

Grading system

Grade	**No. of points**	**Description**
10	91-100	Excellent
9	81-90	Exceptionally good
8	71-80	Very good
7	61-70	Good
6	51-60	Passing
5	<51	Failing

(Table 5.2) Course unit description