



УНИВЕРЗИТЕТ У БАЊОЈ ЛУЦИ
UNIVERSITY OF BANJA LUKA
ПРИРОДНО-МАТЕМАТИЧКИ ФАКУЛТЕТ
FACULTY OF NATURAL SCIENCES AND MATHEMATICS



CHEMISTRY DEPARTMENT

FIRST CYCLE OF STUDY

Chemistry/Chemistry Education

Course name	Computational Chemistry			
Course code	Course status	Semester	Hours of instruction	ECTS
1C16HOS1108	elective	VI	3+0	4
Teacher(s)	Assis. Prof. Danijela Barić PhD			

Prerequisite course(s)	Entry requirements
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Course goals

The aim of the course *Computational Chemistry* is to acquire basic knowledge and skills for the application of computer methods in chemistry, which represent the most modern approach in the design of complex organic molecules of specific stereochemistry and predetermined properties, and study and prediction of chemical reaction mechanisms.

Learning outcomes

Students will be introduced to the principles and methods of computer chemistry, the basics of molecular modeling important for the design of complex organic molecules, computer study of the mechanism of organic reactions and molecule design based on the application of quantum chemical methods.

Course content

Introduction to basic tools needed for chemistry in silico, basic concepts and definitions in computational chemistry, basics of molecular mechanics, minimization method, basics of molecular orbital theory (MO), ab initio MO theory, sets of basic functions, self-consistent field method (SCF) and Hartree -Fock theory, potential energy plane, geometry optimization, transition state localization, electronic correlation problem and post-HF methods, Møller-Plesset perturbation (MP) theory, solvent description, functional density theory (DFT) and application of DFT methods. Examples from the teaching material for active student participation.

Teaching methods

Lectures and calculation exercises

Books and other learning materials

Christopher J. Cremer, **Essentials of Computational Chemistry: Theories and Models**, 2nd Edition, John Wiley & Sons, Chichester, 2004.

Andrew R. Leach, **Molecular Modelling: Principles and Applications**, 2nd Edition, Pearson Education Ltd, 2001. Frank Jensen, **Introduction to Computational Chemistry**, 2nd Edition, John Wiley & Sons, Chichester, 2006.

Teacher's internal script*

Course activities and grading method

The results of the tests are entered in the final grade only if they exceed 50% of the planned points for a given form of test during the semester.

Seminar	40	Final exam	60
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Additional course notes

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Name of the teacher who prepared this form Danijela Barić