|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Study program:** Master studies Chemistry | | | | |
| **Course title:** Computational Chemistry (H223C) | | | | |
| **Name of lecturer/lecturers:** Marija S. Genčić | | | | |
| **Type of course:** compulsory | | | | |
| **Number of ECTS allocated: 4** | | | | |
| **Course objectives:** Obtaining the necessary basic knowledge and skills for the use of various computer methods, as well as the necessity of their application in chemistry. Advanced solving of questions and problems that cannot be solved experimentally, but only with the use of computers. Getting to know the importance of molecular modeling, different computer methods and the possibilities of their application for the study of geometry and optimization of molecules. | | | | |
| **Course outcomes:** Upon successful completion of this course, the student is able to use various computational methods for molecular modeling, learned what chemical informatics is and which problems in chemistry can be solved using an informatics approach. They will acquire skills in using Spartan and Gaussian software packages and independence in modeling various chemical phenomena. | | | | |
| **SYLLABUS**  *Lectures*  Concept of computational chemistry. Programming languages. Computer methods in chemistry. Molecular mechanics - potential energy functions. Molecular mechanics - field of forces. Calculation of molecular geometry, geometry optimization. Methods based on quantum mechanics. Ab initio methods. DFT methods. Comparison of ab initio and DFT methods. Conformational analysis. Molecular dynamics. Molecular recognition, electrostatic potential surface. Chemical informatics. Connecting the structure of molecules and the behavior of substances.  *Laboratory work*  Theoretical exercises. Using Spartan and Gaussian software packages. Molecular mechanics, molecular mechanics methodology, potential energy functions, optimization algorithms, geometry optimization of a large number of molecules, conformational analysis of different molecules. Ab initio methods, application of programs based on ab initio methods. DFT methods and corresponding programs. Application of ab initio and DFT methods for solving problems in chemistry. Basics of programming, algorithm, writing programs to solve some problems in chemistry. Use of chemical informatics methods. Use of data banks. | | | | |
| **References**  1. S. Marković, Z. Marković, Molekulsko modeliranje, Centar za naučno-istraživački rad Srpske akademije nauka i umetnosti i Univerzitet u Kragujevcu, Kragujevac, 2012.  2. M. Zlatanović, D. Petrović, Osnovi molekulskog modelovanja, praktikum, Hemijski fakultet, Univerzitet u Beogradu, 2016.  Pomoćna literatura  3. A. R. Leach, Molecular Modeling – principles and applications, 2nd ed., Pearson Education, 2001.  4. H.-D-Höltje, W. Sippl, D. Rognan, G. Folkers, Molecular Modeling-basic principles and applications, 3rd ed., Wiley-VCH, 2008. | | | | |
| **Active teaching classes** | **Lectures 30** | | **Laboratory work 15** | |
| **Teaching mode:** Lectures, theoretical exercises, seminar work | | | | |
| **ASSESSMENT METHODS AND CRITERIA (Max 100 points)** | | | | |
| **Pre exam duties** | **Points** | **Final exam** | | **Points** |
| Activity during lectures | 5 | Written examination | | 20 |
| Practical teaching | 15 | Oral examination | | 20 |
| Teaching colloquia | 20 |  | |  |
| Seminar | 20 |  | |  |