

## FIȘA DISCIPLINEI

### 1. Data about program

|                                     |                                      |
|-------------------------------------|--------------------------------------|
| 1.1 Institution                     | Babeș-Bolyai University, Cluj-Napoca |
| 1.2 Faculty                         | Chemistry and Chemical Engineering   |
| 1.3 Department                      | Chemistry                            |
| 1.4 Studies domain                  | Chemistry, Chemical Engineering      |
| 1.5 Studies cycle                   | Master                               |
| 1.6 Studies Program / Qualification | ADVANCED CHEMISTRY / master degree   |

### 2. Data about the discipline

|                                  |  |              |   |                         |    |                       |                 |
|----------------------------------|--|--------------|---|-------------------------|----|-----------------------|-----------------|
| 2.1 Name of discipline           | <b>Molecular Modeling and Design – CME7334</b> |              |   |                         |    |                       |                 |
| 2.2 Appointed person for lecture | Assist. Prof. dr. Gabriela Nemeș               |              |   |                         |    |                       |                 |
| 2.3 Appointed person for seminar | Assist. Prof. dr. Gabriela Nemeș               |              |   |                         |    |                       |                 |
| 2.4 Year of studies              | II   | 2.5 Semester | 3 | 2.6. Type of evaluation | VP | 2.7 Discipline regime | SD <sup>a</sup> |

<sup>a</sup>SD = specialized discipline

### 3. Total time estimated (hours per semester, didactic activities)

|   |     |                       |    |                        |    |
|---|-----|-----------------------|----|------------------------|----|
| 3.1 Hours per week  | 3   | Of which: 3.2 lecture | 2  | 3.3 seminar/laboratory | 1  |
| 3.4 Total No. of hours in the studies plan                            | 42  | Of which: 3.5 lecture | 28 | 3.6 seminar/laboratory | 14 |
| Distribution of time :  |     |                       |    |                        | h  |
| Studies upon manual, lecture support, bibliography and personal notes |     |                       |    |                        | 20 |
| Supplementary documentation in library or on specialized websites     |     |                       |    |                        | 20 |
| Preparation of seminars/ themes, reports, essays                      |     |                       |    |                        | 35 |
| Tutorial activities   |     |                       |    |                        | 4  |
| Exams   |     |                       |    |                        | 4  |
| Other: .....  |     |                       |    |                        | -  |
| 3.7 Total hours of individual study                                   | 83  |                       |    |                        |    |
| 3.8 Total hours per semester  | 125 |                       |    |                        |    |
| 3.9 Number of credit points   | 5   |                       |    |                        |    |

### 4. Preliminary conditions (where applied)

|                     |   |
|---------------------|---|
| 4.1 of curricula    | <ul style="list-style-type: none"> <li>no need</li> </ul> |
| 4.2 of competencies | <ul style="list-style-type: none"> <li>no need</li> </ul> |

### 5. Conditions (where applied)

|                                 |  |
|---------------------------------|--|
| 5.1 For lecture                 | <ul style="list-style-type: none"> <li>Students will attend the lectures with their mobile phones on silent mode or turned off.</li> <li>The students will receive printouts of the PowerPoint slides of the lectures before each lecture.</li> </ul>                                |
| 5.2 For seminar/ practical work | <ul style="list-style-type: none"> <li>Students will attend the seminars with their mobile phones on silent mode or turned off.</li> <li>The essays and the laboratory results will be handed out in electronic format and will condition the grading of this discipline.</li> </ul> |

## 6. Specific competences acquired

|                          |  |
|--------------------------|--|
| Professional competences | <ul style="list-style-type: none"> <li>Recognizing and describing the concepts, approaches, theories and methods of molecular modeling.</li> <li>Explaining and interpreting some concepts and chemical proprieties through means of molecular modeling.</li> <li>Applying fundamental notions for solving chemistry problems by employing molecular modeling techniques.</li> </ul>   |
| Crosswise competences    | <ul style="list-style-type: none"> <li>Executing, independently, complex professional duties and autonomously conducting research-design activities, using computer assisted techniques by respecting the professional ethics and moral conduct rules.</li> <li>Planning, monitoring and assuming the professional duties of a subordinate professional group. Proving the ability to coordinate the activity, analytical thinking, adaptability and flexibility, cooperation with the team members.</li> <li>Self-assessment of the own professional performances and establishing the needs of continuous training, informing and constant documentation in their field of work and related fields, as required by the current needs in the labor market.</li> </ul> |

## 7. Specific objectives (pointed out from the acquired competences)

|                         |   |
|-------------------------|---|
| 7.1 General objectives  | <ul style="list-style-type: none"> <li>To become familiar with basic and advanced notions, concepts, theories and basic models in the field of computational chemistry with applications in chemistry and chemical engineering.</li> </ul>  |
| 7.2 Specific objectives | <ul style="list-style-type: none"> <li>Acquiring knowledge to improve the performance of chemical and biochemical processes by employing computer assisted tools and sustainable development principles.</li> <li>Acquiring knowledge to develop and use mathematical models and simulations by using specific software.</li> </ul> |

## 8. Content

| 8.1 Lecture   | Teaching methods   | Notes |
|---|--|-------|
| 8.1.1. Introduction to molecular modeling, definition of the field, its relation to the other chemistry branches. | lecture, explanation, discussion                             |       |
| 8.1.2. Potential Surfaces   | lecture, explanation, discussion                             |       |
| 8.1.3. Molecular Mechanics  | lecture, explanation, discussion                             |       |
| 8.1.4-5. Basis of the molecular orbitals theory   | lecture, explanation, discussion                             |       |
| 8.1.6. <i>Semi-empirical</i> MO methods   | lecture, explanation, discussion                             |       |
| 8.1.7. <i>Ab initio</i> MO methods  | lecture, explanation, discussion                             |       |
| 8.1.8. Post-Hartree-Fock methods  | explanation, discussion, description, brainstorming, debate  |       |
| 8.1.9 Density Functional Theory (DFT)   | lecture, explanation, discussion, description, brainstorming |       |
| 8.1.10. Hybrid QM/MM methods  | lecture, explanation,  |       |

|   |  |  |
|---|--|--|
|   | discussion, description, brainstorming, debate               |  |
| 8.1.11. Calculation of the properties of molecular systems.   | lecture, explanation, discussion, description, brainstorming |  |
| 8.1.12. Calculation of the properties of molecular system: The determining of charge distribution, electrostatic molecular potentials | lecture, explanation, discussion, description, brainstorming |  |
| 8.1.13. Computing of excited states   | lecture, explanation, discussion, description, brainstorming |  |
| 8.1.14. Determining the reaction mechanisms by computing transition states  | lecture, explanation, discussion, description, brainstorming |  |

### References

1. C.J.Cramer, Essentials of Computational Chemistry, Theories and Models, Wiley, 2004.
2. E.Lewars, Computational Chemistry, Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Kluwer Academic Publishers, 2003
3. I.Silaghi-Dumitrescu, D. Horvath, Mecanica Moleculara, Presa Universitara Cluj-Napoca, 1996.
4. F.Jensen, Introduction to Computational Chemistry, Wiley, 1999.

| 8.2 Seminar / laboratory   | Teaching methods   | Observation   |
|--|--|---|
| 8.2.1. Presentation of the practical activities, requirements, manner of preparing the reports. Introduction. Building molecular models using a computer | explanation, discussion, description, brainstorming, experiment  | The practical work will be organized bimonthly, in 2 hour sessions. |
| 8.2.2. Modeling of the molecular structure and energy using <i>ab initio</i> techniques  | experiment, explanation, discussion, description, brainstorming, |   |
| 8.2.3. Modeling of the molecular structure and energy using <i>semiempiric</i> methods   | experiment, explanation, discussion, description, brainstorming  |   |
| 8.2.4. Modeling of complex molecular properties detectable at macroscopic level  | Experiment, explanation, discussion, description, brainstorming, |   |
| 8.2.5. Building models that involve more molecules; supramolecular systems, nanosystems.   | Experiment, explanation, discussion, description, brainstorming, |   |
| 8.2.6. Modeling of chemical reactivity at molecular and supramolecular level   | Experiment, explanation, discussion, description, brainstorming, |   |
| 8.2.7. Modeling of the shape and energy of supramolecular systems and nanosystems. Evaluation.   | Experiment, explanation, discussion, description, brainstorming, |   |

### References

1. W.J. Hehre, A.J. Shusterman, W.W. Huang, A laboratory Book of Computational Organic Chemistry, Wavefunction, Irvine, California, 1996.
2. E.Lewars, Computational Chemistry, Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Kluwer Academic Publishers, 2003
3. Spartan '04. Tutorial and User Guide, Wavefunction, 2003..

**9. Relationship between the content of the specific discipline with the requirements of the epistemic community, professional associations and potential employers.**

- By acquiring the theoretical and applied skills included in the content of the discipline „Molecular modeling and design” the students are acquiring consistent knowledge, corresponding to the competences required for the potential jobs included in diploma supplement and ANC.

**10. Evaluation**

| Type of activity  | 10.1 Evaluation criteria  | 10.2 Evaluation methods   | 10.3 Contribution to the final mark |
|---|---|---|-------------------------------------|
| 10.4 Lecture  | Quality of the given answers – appropriate acquiring and understanding of the subjects presented during the lectures. | Written examination – the grading will be conditioned by the accomplishing the practical work.<br>The intent to defraud will be punished by removal from the exam. The fraud will be punished by expelling, as stipulated in the ECTS rules of UBB. | 80%                                 |
|   | Correct solving of the problems   |   |                                     |
| 10.5 Seminar/laboratory   | Quality of the given answers – appropriate acquiring and understanding of the subjects presented during the seminars. | Grading will be done based on the written reports and supplementary data required as annexes in case of the modeling activities.  | 20%                                 |
|   | Quality of the prepared reports   |   |                                     |
|   | Activity performed in the laboratory  |   |                                     |
| 10.6 Minimum standard of performance  |   |   |                                     |
| <ul style="list-style-type: none"><li>• Mark 5 (five).</li><li>• Knowledge of the introduction notions; use of modeling methods for a material with known chemical composition, identifying of the properties that can be foreseen and the level of precision/utility of the applied methods.</li></ul> |   |   |                                     |

Data completării

13. 04. 2021

Semnătura titularului de curs

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Semnătura titularului de seminar

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Data avizării în departament

13.04.2021

Semnătura directorului de departament

Acad. Cristian Sorin Silvestru

