FIŞA DISCIPLINEI

1. Data about program

1.1 Institution	Babeş-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's degree

2. Data about the discipline

2.1 Name of discipline	**Molecular Modeling and Design – CME7334**						
2.2 Appointed person for lecture	Lect. dr. Ionuț-Tudor Moraru						
2.3 Appointed person for seminar	Lect. dr. Ionuț-Tudor Moraru						
2.4 Year of studies	II	2.5 Semester	3	2.6. Type of evaluation	VP	2.7 Discipline regime	DS

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	2
3.4 Total No. of hours in the studies plan	56	Of which: 3.5 lecture	28	3.6 seminar/laboratory	28
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					20
Tutorial activities					5
Exams					4
Other:					-

3.7 Total hours of individual study	69
3.8 Total hours per semester	125
3.9 Number of credit points	5

4. Preliminary conditions (where applied)

4.1 of curricula	• no need
4.2 of competencies	• no need

5. Conditions (where applied)

5.1 For lecture	• Students will attend the lectures with their mobile phones on silent mode or turned off. • The students will receive printouts of the PowerPoint slides of the lectures before each lecture.
5.2 For seminar/ practical work	• Students will attend the seminars with their mobile phones on silent mode or turned off. • The essays and the laboratory results will be handed out in electronic format and will condition the grading of this discipline.

6. Specific competences acquired

Professional competences	• Recognizing and describing the concepts, approaches, theories and methods of molecular modeling. • Explaining and interpreting some concepts and chemical proprieties through means of molecular modeling. • Applying fundamental notions for solving chemistry problems by employing molecular modeling techniques.
Crosswise competences	• Executing, independently, complex professional duties and autonomous conducting research-design activities, using computer assisted techniques by respecting the professional ethics and moral conduct rules. • 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. • 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.

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

7.1 General objectives	• 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.
7.2 Specific objectives	• Acquiring knowledge to improve the performance of chemical and biochemical processes by employing computer assisted tools and sustainable development principles. • Acquiring knowledge to develop and use mathematical models and simulations by using specific software.

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 Energy Surfaces	lecture, explanation, discussion	
8.1.3. Molecular Mechanics	lecture, explanation, discussion	
8.1.4-5. Basis of the molecular orbital theory	lecture, explanation, discussion	
8.1.6. Semiempirical MO methods	lecture, explanation, discussion	
8.1.7. *Ab initio* MO methods	lecture, explanation, discussion	
8.1.8. Post-Hartee-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. Computing the properties of molecular systems.	lecture, explanation, discussion, description, brainstorming	
8.1.12. Computing the properties of molecular systems: charge distribution, electrostatic molecular potentials	lecture, explanation, discussion, description, brainstorming	
8.1.13. Excited states calculations	lecture, explanation, discussion, description, brainstorming	
8.1.14. Computing the reaction mechanisms; transition state calculations	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 the molecular structure and energy using computational techniques (semiempirical and *ab initio* methods)	experiment, explanation, discussion, description, brainstorming,	
8.2.3. Modeling the molecular structure and energy using computational techniques (*ab initio* and DFT methods)	experiment, explanation, discussion, description, brainstorming	
8.2.4. Modeling complex molecular properties that are detectable at macroscopic level	Experiment, explanation, discussion, description, brainstorming,	
8.2.5. Building models that involve several molecules; supramolecular systems, nanoscale systems.	Experiment, explanation, discussion, description, brainstorming,	
8.2.6. Modeling chemical reactivity at molecular and supramolecular levels	Experiment, explanation, discussion, description, brainstorming,	
8.2.7. Modeling the shape and energy of supramolecular systems and nanostructures. Evaluation of their stability.	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..

4. Referate de laborator – Microsoft Teams

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.	Continuous assessment – the grading will be conditioned by the accomplishment of the practical activities. 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			
• Mark 5 (five). • 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.			

Data completării: 10. 04. 2024

Semnătura titularului de curs

Semnătura titularului de seminar

Data avizării în departament
14.04.2024

Semnătura directorului de departament
Prof. Dr. Habil. Ing. Monica Toșa