

FIȘA DISCIPLINEI

1. Data on the program

1.1 Institution of higher education	Babeș-Bolyai University, Cluj-Napoca
1.2 Faculty	Chemistry and Chemical Engineering
1.3 Department	Chemistry
1.4 Area of study	Chemistry, Chemical Engineering
1.5 Cycle of study	Master
1.6 Study programme / qualification	Advanced Chemistry, Advanced Chemical Process Engineering / Master's Degree

2. Data on the discipline

2.1 Name of the discipline	Molecular modeling and design - CMP6112						
2.2 Lecturer	Conf. dr. Radu Silaghi-Dumitrescu						
2.3 Seminar/laboratory assistant	Asist. Dr. Petronela Maria Petrar						
2.4 Year	II	2.5 Semester	3	2.6. Type of evaluation	E	2.7 Regime of the discipline	Ob/fac

3. Total estimated time (hours per semester for teaching/learning activities)

3.1 Hours per week	3	Of which: 3.2 curs	2	3.3 seminar/laboratory	1
3.4 Total total hours in curriculum	42	Of which: 3.5 curs	28	3.6 seminar/laboratory	14
Distribution of time:					ore
Study using manuals, lecture support, bibliography, notes					20
Additional documentation in the library, on electroinic databases, on field					20
Preparation of seminars/laboratories, homework, essays					60
Tutoring					4
Examination					4
other:					-
3.7 Total hours individual study	108				
3.8 Total hours per semester	150				
3.9 Number of credits	6				

4. Preconditions (if existing)

4.1 de curriculum	• -
4.2 de competențe	• -

5. Conditions (if applicable)

5.1 Lecture	<ul style="list-style-type: none"> • Mobile phones off or silent • Powerpoint printouts distributed to the students in advance
5.2 Seminar/laboratory	<ul style="list-style-type: none"> • Mobile phones off or silent • Homework (written and as attached calculation files) to be turned in electronically, on time

6. Specific competences

Professional competences	<ul style="list-style-type: none"> • Technological design of processes and instruments specific to process engineering for improvement of performance in chemical and biochemical processes using computer-aided design (CAD) and sustainable development principles • Development of mathematical models and of simulations in process engineering, for diagnosing problems, analyzing optimal running conditions, and handling of (bio)chemical processes
transverse competences	<ul style="list-style-type: none"> • Independent completion of complex professional tasks and autonomous conduction of research and design experiments, using computer-aided design and complying with moral and professional ethics standards • Planning, monitoring and endorsement of professional tasks within a hierarchy-bound professional group. Demonstration of abilities to coordinate activities, analytical thinking flexibility, collaboration with team members • Self-evaluation of performance and appraisal of the needs for continuing education, continuing documentation and formation in the respective field of activity and in related fields, in line with the requirements of the labor market

7. Objectives of the discipline

7.1 general objectives	<ul style="list-style-type: none"> • Familiarize students with basic and advanced notions, concepts, theories and basic models in chemistry and chemical engineering
7.2 specific objectives	<ul style="list-style-type: none"> • Acquire knowledge for improving the performance of chemical and biochemical processes using computer-aided design and the principles of sustainable development • Acquire knowledge for using and developing mathematical models and simulations in process engineering, for diagnosing problems, analyzing the optimal working regimes for (bio)chemical processes

8. Content

8.1 Lecture	Teaching methods	Observations
8.1.1. Introduction in molecular modeling; definition of the field; relationship with other branches of chemistry	Lecture; explication; conversation; description	
8.1.2. Potential surfaces	Lecture; explication; conversation; description	
8.1.3. Molecular mechanics	Lecture; explication; conversation; description	
8.1.4-5. Basis of molecular orbital theory.	Lecture; explication; conversation; description	
8.1.6. semiempirical MO methods	Lecture; explication; conversation; description	
8.1.7. ab initio MO methods	Lecture; explication; conversation; description	
8.1.8. post-HF methods	Lecture; explication; conversation; description	

8.1.9. density functional theory (DFT).	Lecture; explication; conversation; description	
8.1.10. hybrid QM/MM methods	Lecture; explication; conversation; description	
8.1.11. excited state calculations	Lecture; explication; conversation; description	
8.1.12. Thermodynamic property calculations	Lecture; explication; conversation; description	
8.1.13. Determination of charge distribution; electrostatic potential surfaces	Lecture; explication; conversation; description	
8.1.14. Determination of reaction mechanisms via transition state calculations	Lecture; explication; conversation; description	
Bibliography		
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	Observații
8.2.1. Presentation of the seminar topics; conditions, requirements for completing assignments. Introductory notions.	Lecture; explication; conversation; description; experiment	
8.2.2. Building molecular models on the computer	Lecture; explication; conversation; description; experiment	
8.2.3. Modeling molecular shape and energy using molecular mechanics	Lecture; explication; conversation; description; experiment	
8.2.4-5. Modeling molecular shape and energy using ab initio and semiempirical methods	Lecture; explication; conversation; description; experiment	
8.2.6. Modeling complex molecular properties detectable at macroscopic level	Lecture; explication; conversation; description; experiment	
8.2.7-8. Building models involving more than one molecule; supramolecular systems, nanosystems	Lecture; explication; conversation; description; experiment	
8.2.9-10. Modeling chemical reactivity at molecular and supramolecular level	Lecture; explication; conversation; description; experiment	
8.2.11-12. Modeling shape and energy in supramolecular and nano systems	Lecture; explication; conversation; description; experiment	
8.2.13. Dynamics techniques	Lecture; explication; conversation; description; experiment	
8.2.14. Evaluation	Test	
Bibliography		
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.		

9. Coroborarea conținuturilor disciplinei cu așteptările reprezentanților comunității epistemice, asociațiilor profesionale și angajatori reprezentativi din domeniul aferent programului

- Prin însușirea conceptelor teoretico-metodologice și abordarea aspectelor practice incluse în disciplina Modelare și design molecular studenții dobândesc un bagaj de cunoștințe consistente, în concordanță cu competențele parțiale cerute pentru ocupațiile posibile prevăzute în Grila 1 – RNCIS.

10. Evaluation

Activity type	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Weight on final grade
10.4 Curs	Correctness of answers – apprehension and comprehension of the issues discussed in the lectures	Written examination – conditioned by completion of the laboratory activities. Attempted fraud is sanctioned by stopping the examination. Fraud is sanctioned by expulsion as per the ECST regulations of BBU	80%
	Correct solving of the problems		
10.5 Seminar/laboratory	Correctness of answers – apprehension and comprehension of the issues discussed in the seminar/laboratory	Grading is based on the completed homework – written as well as in the form of electronic files requested for the modeling activities	20%
	Quality of homework		
	Quality of work during the laboratory/seminar		
10.6 minimal standards of performance			
<ul style="list-style-type: none"> • Grade equal to 5 (five). • Knowledge of introductory notions; application of the modeling methods on a material of known chemical composition, identifying those properties which can be predicted and the level of precision/utility of the applied methods 			

Date

Signature of lecturer

Signature of seminar/laboratory assistant

22 October 2012....

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Date of approval by the department

Signature of department director

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