



UNIVERSITATEA BABES-BOLYAI
BABES-BOLYAI TUDOMÁNYEGYETEM
BABES-BOLYAI UNIVERSITAT
BABES-BOLYAI UNIVERSITY
TRADITIO ET EXCELLENTIA

Tradiție și Excelență prin
Cultură - Știință - Inovație din 1581



Facultatea de Chimie și Inginerie Chimică

Str. Arany János nr. 11
Cluj-Napoca, cod poștal 400028
Tel.: 0264-59.38.33
Fax: 0264-59.08.18

secretariat.chem@ubbcluj.ro
www.chem.ubbcluj.ro

SYLLABUS


Molecular Modeling and Design

University year: 2025-2026

1. Information regarding the programme

1.1. Higher education institution	Babes-Bolyai University, Cluj Napoca
1.2. Faculty	Faculty of Chemistry and Chemical Engineering
1.3. Department	Chemistry
1.4. Field of study	Chemical Engineering
1.5. Study cycle	Master
1.6. Study programme/Qualification	Advanced Chemical Process Engineering
1.7. Form of education	Full-time education

2. Information regarding the discipline

2.1. Name of the discipline			Molecular Modeling and Design				Discipline code		CME7334		
2.2. Course coordinator			Lect. dr. Ionuț-Tudor Moraru								
2.3. Seminar coordinator			Lect. dr. Ionuț-Tudor Moraru								
2.4. Year of study		II	2.5. Semester		3	2.6. Type of evaluation		VP	2.7. Discipline regime		DS

3. Total estimated time (hours/semester of didactic activities)

3.1. Hours per week	4	of which: 3.2 course	2	3.3 seminar/laboratory	2
3.4. Total hours in the curriculum	56	of which: 3.5 course	28	3.6 seminar/laborator	28
Time allotment for individual study (ID) and self-study activities (SA)					hours
3.5.1. Learning using manual, course support, bibliography, course notes (SA)					20
3.5.2. Additional documentation (in libraries, on electronic platforms, field documentation)					15
3.5.3. Preparation for seminars/labs, homework, papers, portfolios and					20
3.5.4. Tutorship					5
3.5.5. Evaluations					4
3.5.6. Other activities:					5
3.7. Total individual study hours	69				
3.8. Total hours per semester	125				
3.9. Number of ECTS credits	5				



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4. Prerequisites (if necessary)

4.1. curriculum	• no need
4.2. competencies	• no need

5. Conditions (if necessary)

5.1. for the course	<ul style="list-style-type: none"> • 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 the seminar /lab activities	<ul style="list-style-type: none"> • 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 competencies acquired

Professional/essential competencies	<ul style="list-style-type: none"> • 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.
Transversal competencies	<ul style="list-style-type: none"> • 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.
Responsibility and autonomy:	<ul style="list-style-type: none"> • The student has the ability to work independently in order to fulfill complex professional duties and autonomous conducting research-design activities, using computer assisted techniques by respecting the professional ethics and moral conduct rules.

7. Objectives of the discipline (outcome of the acquired competencies)

7.1 General objective of the discipline	<ul style="list-style-type: none"> • 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.
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7.2 Specific objective of the discipline	<ul style="list-style-type: none"> 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.
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8. Content

8.1 Course	Teaching methods	Remarks
8.1.1. Introduction to molecular modeling; definition of the field, and correlation with other branches of chemistry.	lecture, explanation, discussion	2h
8.1.2. Potential Energy Surfaces (PES).	lecture, explanation, discussion	2h
8.1.3. Molecular Mechanics (MM).	lecture, explanation, discussion	2h
8.1.4-5. Molecular orbital (MO) theory; MO diagrams for A_2 , AB and AB_n ($n \geq 2$) systems.	lecture, explanation, discussion	2h
8.1.6. Basis sets.	lecture, explanation, discussion	2h
8.1.7. Hückel Theory; Semiempirical methods.	lecture, explanation, discussion	2h
8.1.8. <i>Ab initio</i> calculations; the Hartree-Fock (HF) method.	lecture, explanation, discussion	2h
8.1.9. Post-Hartree-Fock methods.	lecture, explanation, discussion	2h
8.1.10 Density Functional Theory (DFT).	lecture, explanation, discussion	2h
8.1.11. Hybrid QM/MM methods.	lecture, explanation, discussion	2h
8.1.12.-13. Computing the properties of molecular and supramolecular systems: charge distribution, electrostatic molecular potentials, vibrational frequencies, <i>etc.</i>	lecture, explanation, discussion	2h
8.1.14. Excited states calculations; the time-dependent (TD) DFT method; applications in UV-Vis and CD spectroscopy.	lecture, explanation, discussion	2h

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	Remarks
8.2.1. Presentation of the practical activities, requirements, and manner of preparing the reports. Introduction. Building molecular models using <i>GaussView</i> software.	explanation, discussion, description, brainstorming, experiment	The practical work will be organized bimonthly, in 4 hour sessions.
8.2.2. Modeling the structure of several molecular systems using <i>ab-initio</i> and semiempirical methods; analysis of the relative energy: case study on the cyclohexane ring.	experiment, explanation, discussion, description, brainstorming,	
8.2.3. Geometry optimizations of several metal complexes and clusters; DFT techniques.	experiment, explanation, discussion, description,	



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	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 and nanoscale systems. Computing the strength of secondary interactions (e.g., hydrogen bonds, metal- π interactions, <i>etc.</i>).	Experiment, explanation, discussion, description, brainstorming,	
8.2.6. Modeling chemical reactivity; reactions mechanisms; transition states.	Experiment, explanation, discussion, description, brainstorming,	
8.2.7. Computing the UV-Vis spectra of several chromophore systems via TD-DFT calculations.	Experiment, explanation, discussion, description, brainstorming,	
Bibliography 1. W. J. Hehre, A. J. Shusterman, W. W. Huang, <i>A laboratory Book of Computational Organic Chemistry</i> , Wavefunction, Irvine, California, 1996. 2. E. Lewars, <i>Computational Chemistry, Introduction to the Theory and Applications of Molecular and Quantum Mechanics</i> , Kluwer Academic Publishers. 2003.		

9. Corroborating the content of the discipline with the expectations of the epistemic community, professional associations and representative employers within the field of the program

- 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

Activity type	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Percentage of final grade
10.4 Course	Quality of the given answers – appropriate acquiring and understanding of the subjects presented during the lectures.	Written examination – the grading will be conditioned by accomplishing the practical work. 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.	70%
	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 oral presentations based on the obtained data.	30%
	Quality of the prepared reports		



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	Activity performed in the laboratory		
10.6 Minimum standard of performance			
<ul style="list-style-type: none">• 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.			

Date:
15.03.2025

Signature of course coordinator

Signature of seminar coordinator

Date of approval:
15.04.2025

Signature of the head of department