COURSE DESCRIPTION

Molecular Modeling and Design

University year: 2026-2027

1. Programme-related data

1.1. Higher Education Institution	Universitatea Babeş-Bolyai din Cluj Napoca
1.2. Faculty	Chemistry and Chemical Engineering
1.3. Department	Chemistry
1.4. Field	Chemistry, Chemical Engineering
1.5. Level of study	Master
1.6. Degree programme / Qualification	ADVANCED CHEMISTRY/master's degree
1.7. Form of education	Full time

2. Course-related data

2.1. Course title	**Molecular Modeling and Design**			Course 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		2.5. Semester		2.6. Type of assessment	Progress check
2.7. Course status	Optional			2.8. Course type	Specialisation subject

3. Total estimated time (hours per semester of teaching activities)

3.1. Number of hours per week	**4**	of which: 3.2. course	**2**	3.3. seminar/ laboratory/ project	**2**
3.4. Total of hours in the curriculum	**56**	of which: 3.5. course	**28**	3.6. seminar/ laboratory	**28**
Time allocation for individual study (IS) and self-taught activities (ST)					**hours**
Learning from textbooks, course materials, bibliography, and notes (IS)					20
Additional research in the library, on subject-specific electronic platforms, and on-site					20
Preparing seminars/ laboratories/ projects, assignments, reports, portfolios, and essays					20
Tutoring (professional guidance)					5
Examinations					4
Other activities					5
3.7. Total hours of individual study (IS) and self-taught activities (ST)				**74**	
3.8. Total hours per semester				**130**	
3.9. Number of credits				**5**	

4. Prerequisites (where applicable)

4.1. curriculum-related	• no need
4.2 skills-related	• no need

5. Specific conditions (where applicable)

5.1. course-related	Interactive participation is encouraged. Materials and useful information will be provided to support the activities. The course will take place on-site at the Faculty of Chemistry and Chemical Engineering. The use of phones or other electronic devices is allowed only for course-related activities.
5.2. seminar/laboratory-related	Attendance at seminar activities is mandatory under the conditions established by the regulations. Completing and submitting seminar assignments will be done according to the schedule set at the

	beginning of the semester, by mutual agreement between the instructor and students. The use of phones or other electronic devices is allowed only for seminar-related activities.

6.1. Competencies resulting from the completion of the degree programme *(as referred to in the curriculum)*[1]

Professional competencies	
Competency code	**Competency**
PC1	Formulating solutions to complex problems in theoretical chemistry and using molecular modeling techniques in the study of chemical and biochemical systems, based on the knowledge and application of advanced concepts and methods from quantum and computational chemistry.
PC2	Description and use of advanced molecular modeling techniques employed to identify and explain the electronic structure, geometry, reaction mechanisms, and spectroscopic properties of molecular systems and nanoparticles.
Transversal competencies	
Competency code	**Competency**
TC3	Designing, planning and performing an individual scientific, multidisciplinary research project.

6.2. Learning outcomes relevant to the degree programme (as referred to in the curriculum)[2]

Learning outcomes targeted by the subject		
Competency code	**Knowledge and comprehension**	**Specific academic skills**
PC1	Formulating solutions to complex problems in theoretical chemistry and applying molecular modelling in chemical and biochemical systems, based on the knowledge, identification, and application of advanced concepts, methods, and theories from computational chemistry	Application of modern methods and techniques from computational chemistry in the study of chemical and biochemical systems
TC3	Knowledge of scientific research strategies, setting the program of experiments and simulations, explanation and interpretation of the results for the elaboration of research projects	Use of fundamental and applied concepts of scientific investigation in order to develop research projects for the development of new technologies

7. Subject-specific learning outcomes

Knowledge and comprehension
The student knows advanced concepts and theories of computational chemistry and their application in the fields of chemistry, biology, and nanotechnology.
The student knows and understands complex issues related to the chemical structure of molecular and nanometric systems being analyzed.
The student works with new concepts and theories related to the modeling and theoretical analysis of complex chemical and biochemical systems.
Specific academic skills
The student analyzes and applies advanced concepts and theories regarding the molecular modeling of complex systems.

[1] The professional and/or transversal skills targeted by the subject for which the course description is prepared will be copied from the curriculum of the degree programme. For each competency, the complete entry, including the competency code, will be copied with the exact wording that appears in the curriculum, without any changes. If no competency is copied from either of the two categories, the row corresponding to that category is deleted from the table.

[2] The learning outcomes relevant for the degree programme and targeted by the subject for which the course description is prepared will be listed. The entries, copied without any changes from the Curriculum by subject type (Core Subject/Specialisation Subject/Complementary Subject), are listed under the corresponding competency.

The student uses computational chemistry techniques creatively in the rational design of new chemical systems.
The student understands and evaluates the spectral properties of complex systems based on molecular modelling techniques.

8. Contents

8.1. Course	**Teaching and learning methods**	**Remarks**[3]
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. *Ab initio* calculations; the Hartree-Fock (HF) method.	lecture, explanation, discussion	2h
8.1.9. Post-Hartee-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, *etc.*	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 and learning methods**	**Remarks**
8.2.1. Presentation of the practical activities, requirements, and manner of preparing the reports. Introduction. Building molecular models using *GaussView* 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 *ab-initio* and semiempirical methods; analysis of the relative energy: case study on the cyclohexane ring.	experiment, explanation, discussion, description, brainstorming,	

[3] For example, organisational aspects, recommendations for students, specific aspects relating to the course/seminar, such as inviting experts in the field, etc.

8.2.3. Geometry optimizations of several metal complexes and clusters; DFT techniques.	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 and nanoscale systems. Computing the strength of secondary interactions (e.g., hydrogen bonds, metal-π interactions, *etc.*).	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, *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.

9. Evaluation

Type of activity	9.1 Evaluation criteria[4]	9.2 Evaluation methods[5]	9.3 Percentage in the final grade
9.4. Course	Quality of the given answers – appropriate acquiring and understanding of the subjects presented during the lectures. Correct solving of the problems	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%
9.5. Seminar/ laboratory	Quality of the given answers – appropriate acquiring and understanding of the subjects presented during the seminars. Quality of the prepared reports Activity performed in the laboratory	Grading will be done based on the written reports and oral presentations based on the obtained data.	30%

9.6 Minimum standard for passing

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.

[4] The evaluation criteria must directly reflect the learning outcomes targeted at the level of the degree programme respectively at the level of the subject. More specifically, the learning outcomes set out in the expected learning outcomes are assessed.

[5] Both final evaluation methods and ongoing evaluation strategies should be established.

10. SDG labels (Sustainable Development Goals)[6]

	○	Sustainable Development Generic Label						
								
○	○	○	●	○	○	○	○	○
								No label applies
○	○	○	○	○	○	○	○	○

Date of entry:
17.04.2026

Signature of course coordinator

Lect. dr. Ionuț-Tudor Moraru

Signature of seminar coordinator

Lect. dr. Ionuț-Tudor Moraru

Date of approval in the department:
24.04.2026

Signature of the head of department

Prof. Habil. Dr. Ing. Monica Ioana Toșa

[6] Select a single label which, according to the *Implementation of SDG labels in the academic process*, best matches the subject. If the subject addresses sustainable development in a generic manner (i.e. by presenting/introducing the general framework of sustainable development, etc.), then the Sustainable Development generic label may be applied. If none of the labels describe the subject, select the last option: *"No label applies."*