COURSE DESCRIPTION

Computational Chemistry

Academic year 2025-2026

1. Programme-related data

1.1. Higher Education Institution	Babeș-Bolyai University, Cluj-Napoca
1.2. Faculty	Chemistry and Chemical Engineering
1.3. Department	Doctoral School of Chemistry
1.4. Field	Chemistry
1.5. Level of study	Doctorate
1.6. Degree programme / Qualification	Doctorate /Doctor in Chemistry
1.7. Form of education	Full time

2. Course-related data

2.1. Course title	**Computational Chemistry**			Course code	**SDC-19-10**
2.2. Course coordinator	Conf. dr. Alexandru Lupan				
2.3. Seminar coordinator	Conf. dr. Alexandru Lupan				
2.4. Year of study	1	2.5. Semester	2	2.6. Type of assessment	Exam
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	**3**	of which: 3.2. course	**1**	3.3. seminar/ laboratory/ project	**2**
3.4. Total of hours in the curriculum	**36**	of which: 3.5. course	**12**	3.6. seminar/ laboratory	**24**
Time allocation for individual study (IS) and self-taught activities (ST)					**hours**
Learning from textbooks, course materials, bibliography, and notes (IS)					40
Additional research in the library, on subject-specific electronic platforms, and on-site					40
Preparing seminars/ laboratories/ projects, assignments, reports, portfolios, and essays					40
Tutoring (professional guidance)					10
Examinations					4
Other activities					-
3.7. Total hours of individual study (IS) and self-taught activities (ST)				**214**	
3.8. Total hours per semester				**250**	
3.9. Number of credits				**10**	

4. Prerequisites (where applicable)

4.1. curriculum-related	Not the case
4.2 skills-related	Not the case

5. Specific conditions (where applicable)

5.1. course-related	
5.2. seminar/laboratory-related	

6.1. Competencies resulting from the completion of the degree programme[1]

[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.

Professional competencies	
Competency code	**Competency**
PC1	Definition of notions, concepts, theories and advanced models in the field of Computational Chemistry as well as their proper use within the professional community
PC4	Use of in-depth knowledge of chemistry to explain and interpret tools and processes specific to computational chemistry
PC5	Identifying and applying advanced concepts, methods and theories to solve problems specific to computational chemistry
Transversal competencies	
Competency code	**Competency**
TC2	Execution of the requested tasks according to the specified requirements and within the imposed deadlines, in compliance with the norms of professional ethics and moral conduct, following a pre-established work plan
TC3	Solving the requested tasks in accordance with the general objectives established by integration within a working group

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	Advanced and up-to-date knowledge in chemistry and the research field; critical understanding of the scientific literature.	Applies and synthesizes advanced concepts/theories to formulate research hypotheses; justifies the choice of scientific approaches.
PC4	Advanced research methodologies: experimental design, modern synthesis and characterization techniques, analysis and validation; principles of research project management.	Designs, plans and implements a research project; applies quality and safety procedures and documents stages and data with full traceability.
PC5	Advanced strategies for data analysis, interpretation, and integration; evaluation of methodological limitations, reproducibility, and scientific impact.	Critically analyses complex data, estimates uncertainty and formulates conclusions; proposes methodological improvements and directions for research/innovation.
TC2	Scientific terminology and communication in Romanian and English; the structure of scientific articles and presentations; good citation practices.	Writes and presents scientific results in Romanian/English coherently; provides well-argued responses to comments and peer reviews.
TC3	Digital tools for research, citation, and data processing (databases, specialized software, reference managers); responsible use of digital resources.	Uses discipline-specific digital tools effectively; manages citations; uses digital resources responsibly in research activities.

7. Subject-specific learning outcomes

Knowledge and comprehension
1. Applying concepts and theories in the field of computational chemistry to develop projects and solve problems
2. Ability to understand and interpret complementary data for the characterization of compounds and chemical processes, to express and argue the interpretation of data based on the correlation of results and comparison with data from the literature
3. Critical analysis and use of advanced methods and techniques for the quantitative and qualitative evaluation of the notions of computational chemistry

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.

4. ...
Specific academic skills
1. Execution of the requested tasks according to the specified requirements and within the imposed deadlines, in compliance with the norms of professional ethics and moral conduct, following a pre-established work plan
2. Concern for improving the results of professional activity by getting involved in the activities carried out
3. Ability to prepare written reports and to publicly defend/support these reports

8. Contents

8.1. Course	**Teaching and learning methods**	**Remarks[3]**
8.1.1. Introduction to computational chemistry, defining the field, the relationship with the other branches of chemistry	Presentation; Explanation, Conversation; Description; Debate	
8.1.2. Potential Energy surfaces	Presentation; Explanation, Conversation; Description; Debate	
8.1.3. Molecular mechanics	Presentation; Explanation, Conversation; Description; Debate	
8.1.4. Molecular orbitals	Presentation; Explanation, Conversation; Description; Debate	
8.1.5. Semiempirical MO methods	Presentation; Explanation, Conversation; Description; Debate	
8.1.6. Ab initio and post-Hartree-Fock MO methods	Presentation; Explanation, Conversation; Description; Debate	
8.1.7. Density functional theory (DFT)	Presentation; Explanation, Conversation; Description; Debate	
8.1.8. Hybrid QM/MM methods	Presentation; Explanation, Conversation; Description; Debate	
8.1.9. Spectroscopic properties	Presentation; Explanation, Conversation; Description; Debate	
8.1.10. Determining charge distributions; molecular electrostatic potentials	Presentation; Explanation, Conversation; Description; Debate	
8.1.11-12. Applications in medicinal chemistry	Presentation; Explanation, Conversation; Description; Debate	
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. L. Piela, Ideas of Quantum Chemistry, 2nd edition, Elsevier, 2014. 5. A. Lupan, A.M.V. Brânzanic, R. Silaghi-Dumitrescu, Elemente de chimie computațională, Presa Universitară Clujeană, Cluj-Napoca, 2024		
8.2. Seminar/ laboratory	**Teaching and learning methods**	**Remarks**
8.2.1. Software packages in computational chemistry; basics of file architecture and manipulation	Conversation, Learning by discovery, Problem solving	
8.2.2-3. Construction, editing, import, export of models / (bio) molecules; quality criteria	Conversation, Learning by discovery, Problem solving	
8.2.4. Types of calculations and methods in the most common software packages; choosing the calculation methodology	Conversation, Learning by discovery, Problem solving	

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

8.2.5-6. Single-point calculations, geometry optimizations, conformation elements; criteria for judging the success of the procedure	Conversation, Learning by discovery, Problem solving	
8.2.7-8. Calculations of molecular and supramolecular properties	Conversation, Learning by discovery, Problem solving	
8.2.9-10. Calculations of reactivity and transition states	Conversation, Learning by discovery, Problem solving	
8.2.11-12 Calculations of biological systems, active sites	Conversation, Learning by discovery, Problem solving	

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.
5. A. Lupan, A.M.V. Brânzanic, R. Silaghi-Dumitrescu, Elemente de chimie computațională, Presa Universitară Clujeană, Cluj-Napoca, 2024.
6. A. Lupan, A. Attia, Sz. Jákó, A.-Z.s Kun, R. B. King, Beyond the Wade-Mingos rules: deviations from sphericality in metallaborane structures, Structure and Bonding, 2021, 139.
7. H. Casian, A. Lupan, R. B. King, High-spin face-capped deltahedra in divanadadicarbaboranes are very different from the singlet structures of chromium analogues. Dalton Trans., 2025, 54, 12463.
8. N. Garrido, A. Pitto-Barry, J. J Soldevila-Barreda, A. Lupan, L. C. Boyes, W. Martin, N. Barry, The sound of chemistry: translating infrared wavenumbers into musical notes, J. Chem. Educ., 2020, 97, 703.

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	Correctness of answers –proper understanding and learning of notions and concepts discussed during lectures; Correct use of learned concept within new contexts. Correct solving of the problems as part of the examination subjects	Written report with interpretation of practical work	50%
9.5. Seminar/ laboratory	Correctness of answers –proper understanding and learning of notions and concepts discussed during lectures; Correct use of learned concept within new contexts. Quality of reports	Written report with interpretation of practical work	50%
9.6 Minimum standard for passing Adequate knowledge of at least one technique for each module.			

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

		Sustainable Development Generic Label

[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.

[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."*

								
			x					
								No label applies

Date of entry:
28.01.2026

Signature of course coordinator

Signature of seminar coordinator

Date of approval in CDSC:

Signature of the Director of the DSC

Prof. dr. Niculina Daniela Hădade